

Supporting Information for

KOt-Bu-Catalyzed Dehydrogenative C–H Silylation of Heteroaromatics: A Combined Experimental and Computational Mechanistic Study

Wen-Bo Liu^{†,‡}, David P. Schuman^{†,‡}, Yun-Fang Yang^{‡,‡}, Anton A. Toutov[†], Yong Liang[‡], Hendrik F. T. Klare[‡], Nasri Nesnas[§], Martin Oestreich[‡], Donna G. Blackmond[‡], Scott C. Virgil[†], Shibdas Banerjee[‡], Richard N. Zare[‡], Robert H. Grubbs[†], K. N. Houk^{‡,*}, and Brian M. Stoltz^{†,*}

[†]*Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, California 91125 United States*

[‡]*Department of Chemistry and Biochemistry, University of California, Los Angeles, California 90095 United States*

[‡]*Institut für Chemie, Technische Universität Berlin, Strasse des 17. Juni 115, 10623 Berlin, Germany*

[§]*Department of Chemistry, Florida Institute of Technology, 150 West University Boulevard, Melbourne, Florida 32901 United States*

[‡]*Department of Chemistry, Stanford University, Stanford, California 94305 United States*

[‡]*Department of Chemistry, The Scripps Research Institute, La Jolla, California 92037 United States*

*houk@chem.ucla.edu;

*stoltz@caltech.edu

[#]These authors contributed equally to this work

Table of Contents:

Materials and Methods	S3
Computational details	S4
Calculated energies and free energy profiles for selected substrates	S5
¹H NMR concentration dependence of silylation product 2	S10
General method for the screening of base catalysts and kinetic profile	S11

Procedure for time course reaction monitoring by in situ ^1H NMR.....	S11
Procedure for time course reaction monitoring by GC analysis of reaction aliquots.....	S13
Procedure for regioselectivity and reversibility of silylation experimentation	S14
General procedure of gas collection by eudiometry	S16
Procedure for silylation reaction in the presence of TEMPO.....	S17
Effect of additives on the silylation reaction	S19
Procedure for reactions using chemical generation of <i>tert</i> -butoxyl radical	S20
Procedure for reaction time course using ReactIR.....	S21
General procedure of ATR-FTIR measurment.....	S22
Procedure for kinetic isotope effect	S23
Procedure for the acquisition of electron paramagnetic resonance (EPR) spectra.	S23
Procedure for reaction calorimetry	S24
General procedure for KO t -Bu-catalyzed silylation and characterization data of new compounds.	S27
EPR Spectrum	S52
^1H NMR and ^{13}C NMR Spectra.....	S53
Zero-point correction (ZPE), thermal correction to energy (ΔE), thermal correction to enthalpy (ΔH), thermal correction to Gibbs free energy (ΔG), energies (E), enthalpies (H), and Gibbs free energies (G) (in Hartree) of the structures calculated at the M06-2X/6-311+G(d,p)-CPCM(THF)//B3LYP/6- 31G(d) level of theory.....	S75
Cartesian coordinates of the structures	S77

Materials and Methods

Unless otherwise stated, reactions were performed in a nitrogen-filled glovebox or in flame-dried glassware under an argon or nitrogen atmosphere using dry, deoxygenated solvents. Solvents were dried by passage through an activated alumina column under argon.¹ Reaction progress was monitored by thin-layer chromatography (TLC), GC or Agilent 1290 UHPLC-MS. TLC was performed using E. Merck silica gel 60 F254 precoated glass plates (0.25 mm) and visualized by UV fluorescence quenching, *p*-anisaldehyde, or KMnO₄ staining. Silicycle SiliaFlash® P60 Academic Silica gel (particle size 40–63 nm) was used for flash chromatography. ¹H NMR spectra were recorded on Varian Inova 500 MHz or Bruker 400 MHz spectrometers and are reported relative to residual CHCl₃ (δ 7.26 ppm), C₆H₆ (δ 7.16 ppm), or THF (δ 3.58, 1.72 ppm). ¹³C NMR spectra were recorded on a Varian Inova 500 MHz spectrometer (125 MHz) or Bruker 400 MHz spectrometers (100 MHz) and are reported relative to CHCl₃ (δ 77.16 ppm). Data for ¹H NMR are reported as follows: chemical shift (δ ppm) (multiplicity, coupling constant (Hz), integration). Multiplicities are reported as follows: s = singlet, d = doublet, t = triplet, q = quartet, p = pentet, sept = septuplet, m = multiplet, br s = broad singlet, br d = broad doublet, app = apparent. Data for ¹³C NMR are reported in terms of chemical shifts (δ ppm). IR spectra were obtained by use of a Perkin Elmer Spectrum BXII spectrometer or Nicolet 6700 FTIR spectrometer using thin films deposited on NaCl plates and reported in frequency of absorption (cm⁻¹). GC-FID analyses were obtained on an Agilent 6850N gas chromatograph equipped with a HP-1 100% dimethylpolysiloxane capillary column (Agilent). GC-MS analyses were obtained on an Agilent 6850 gas chromatograph equipped with a HP-5 (5%-phenyl)-methylpolysiloxane capillary column (Agilent). High resolution mass spectra (HRMS) were obtained from Agilent 6200 Series TOF with an Agilent G1978A Multimode source in electrospray ionization (ESI+), atmospheric pressure chemical ionization (APCI+), or mixed ionization mode (MM: ESI-APCI+), or obtained from Caltech mass spectrometry laboratory. FT-ATR IR measurements were carried out on a Thermo Scientific Nicolet

¹ A. M. Pangborn, M. A. Giardello, R. H. Grubbs, R. K. Rosen and F. J. Timmers, *Organometallics*, **1996**, *15*, 1518.

iS 5 FT-IR spectrometer equipped with an iD5 ATR accessory. ReactIR measurements were carried out on a Mettler-Toledo ReactIR ic10 using a K4 conduit with a Sentinel high-pressure probe and SiComp window. Electron paramagnetic resonance (EPR) spectra were acquired on a X-band Bruker EMX spectrometer. An Omnical SuperCRC or Insight CPR 220 reaction calorimeter were used to monitor heatflow.

Triethyl silane (99%, Sure/Seal™) and KO^t-Bu (sublimed grade, 99.99% trace metals basis) were purchased from Aldrich and used directly. KOH was pulverized and dried in a desiccator over P₂O₅ under vacuum for 24 h prior to use. Di-tert-butyl hyponitrite was synthesized according to literature procedure.² Other reagents were purchased from Sigma-Aldrich, Acros Organics, Strem, or Alfa Aesar and used as received unless otherwise stated.

Computational details

All the calculations were carried out with Gaussian 09.³ Geometry optimization and energy calculations were performed with the B3LYP method⁴ using the 6-31G(d) basis set⁵ for all atom. Frequency analysis verified that the stationary points were minima or first-order saddle points. Single point energies were calculated at the M06-2X⁶/6-311+G(d,p) level with solvent effects (solvent = THF) modeled using the CPCM⁷

² (a) Banks, J. T.; Scaiano, J. C.; Adam, W.; Oestrich, R. S. *J. Am. Chem. Soc.* **1993**, 115, 2473. (b) Mendenhall, G. D. *Tetrahedron Lett.* **1983**, 24, 451.

³ Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09, Rev. D.01*; Gaussian, Inc., Wallingford, CT, 2010.

⁴ (a) Lee, C.; Yang W.; Parr, R. G. *Phys. Rev. B* **1988**, 37, 785. (b) Becke, A. D. *J. Chem. Phys.* **1993**, 98, 1372. (c) Becke, A. D. *J. Chem. Phys.* **1993**, 98, 5648. (d) Stephens, P. J.; Devlin, F. J.; Chabalowski, C. F.; Frisch, M. J. *J. Phys. Chem.* **1994**, 98, 1623.

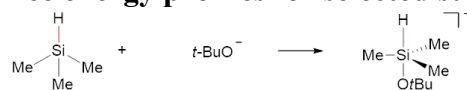
⁵ (a) Ditchfield, R.; Hehre, W. J.; Pople, J. A. *J. Chem. Phys.* **1971**, 54, 724. (b) Hehre, W. J.; Ditchfield, R.; Pople, J. A. *J. Chem. Phys.* **1972**, 56, 2257. (c) Hariharan, P. C.; Pople, J. A. *Theor. Chim. Acta.* **1973**, 28, 213.

⁶ Zhao, Y.; Truhlar, D. *Theor. Chem. Acc.* **2008**, 120, 215.

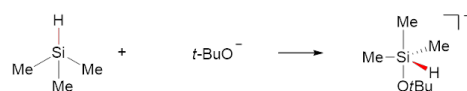
⁷ (a) Barone, V.; Cossi, M. *J. Phys. Chem. A* **1998**, 102, 1995. (b) Cossi, M.; Rega, N.; Scalmani, G.; Barone, V. *J. Comput. Chem.* **2003**, 24, 669. (c) Takano, Y.; Houk, K. N. *J. Chem. Theory Comput.* **2005**, 1, 70.

solvation model. Gibbs free energies in THF at 298.15 K were calculated by adding the thermochemical quantities derived from the B3LYP frequency calculation to the M06-2X solution-phase electronic potential energy. Computed structures are illustrated using CYLVIEW.⁸

Calculated energies and free energy profiles for selected substrates



M062X	6-31G(d)	6-311+G(d,p)	6-311+G(2d,p)	6-311+G(2d,2p)	6-311+G(3df,2p)
ΔG_{gas} (kcal/mol)	-17.5	-8.2	-6.7	-7.2	-9.9
ΔG_{sol} (kcal/mol)	-5.3	7.0	8.2	7.7	4.7
IR(HSiMe ₃) (cm ⁻¹)	2242	2224	2218	2215	2213
IR([HSiMe ₃ Ot-Bu] ⁻) (cm ⁻¹)	1594	1542	1551	1554	1514
IR shift calc. (cm ⁻¹)	648	682	667	661	699



M062X	6-31G(d)	6-311+G(d,p)	6-311+G(2d,p)	6-311+G(2d,2p)	6-311+G(3df,2p)
ΔG_{gas} (kcal/mol)	-18.9	-9.1	-10.8	-10.1	
ΔG_{sol} (kcal/mol)	-4.4	8.3	6.4	7.1	
IR(HSiMe ₃) (cm ⁻¹)	2242	2224	2218	2215	2213
IR([HSiMe ₃ Ot-Bu] ⁻) (cm ⁻¹)	2005	2027	2027	2019	
IR shift calc. (cm ⁻¹)	237	197	191	196	

Figure S1.

Calculated energetics of formation of pentacoordinate silicates their IR spectra of Si-H bonds. The distances of Si-H are shown in angstrom.

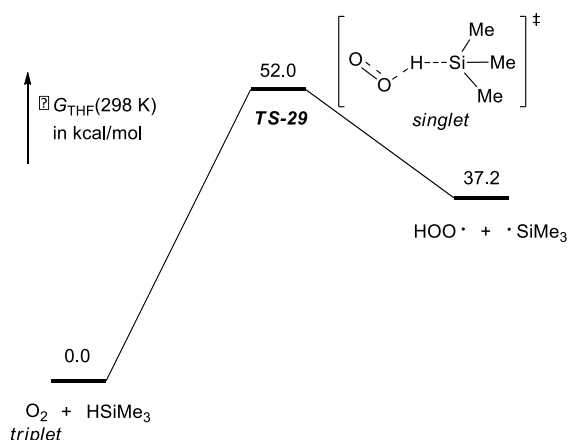


Figure S2.

Free energy profile for generation of silyl radical with oxygen.

⁸ Legault, C. Y. CYLView, 1.0b; Université de Sherbrooke, Canada, **2009**; <http://www.cylview.org>.

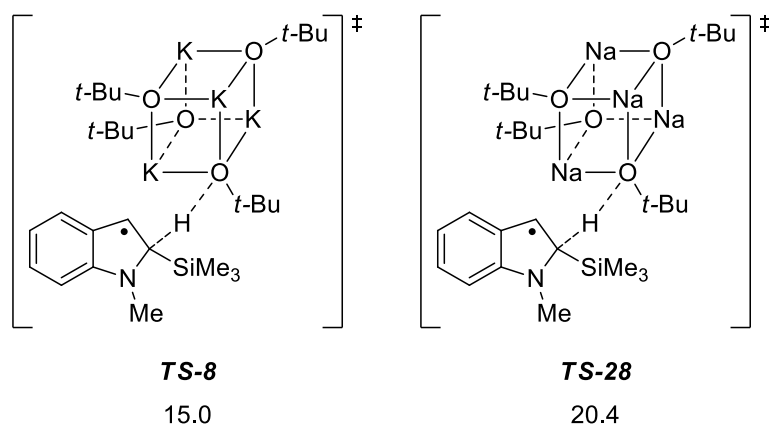


Figure S3.

Transition structures of hydrogen abstraction by tetrameric $(KOt-Bu)_4$ and $(NaOt-Bu)_4$.

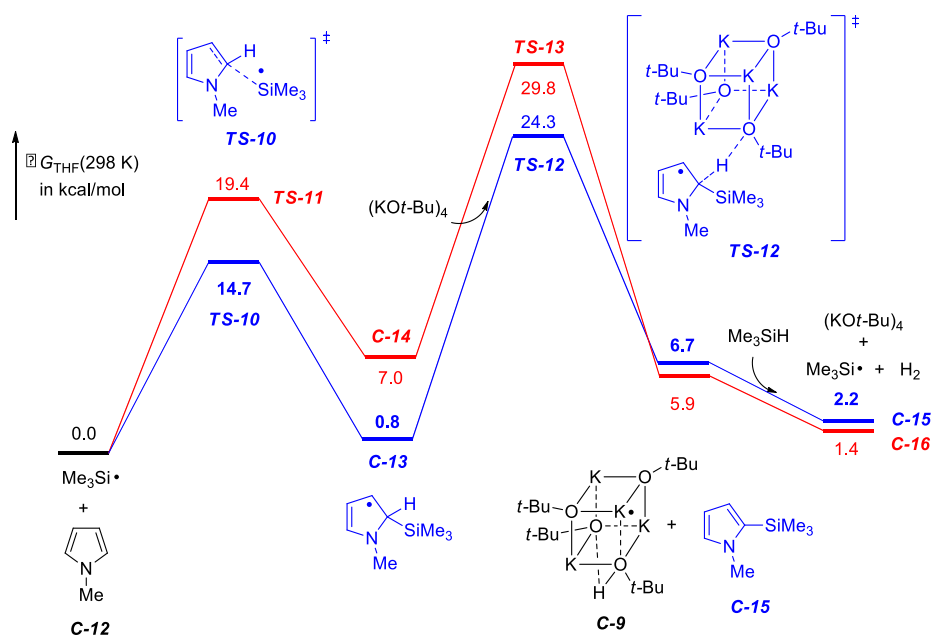
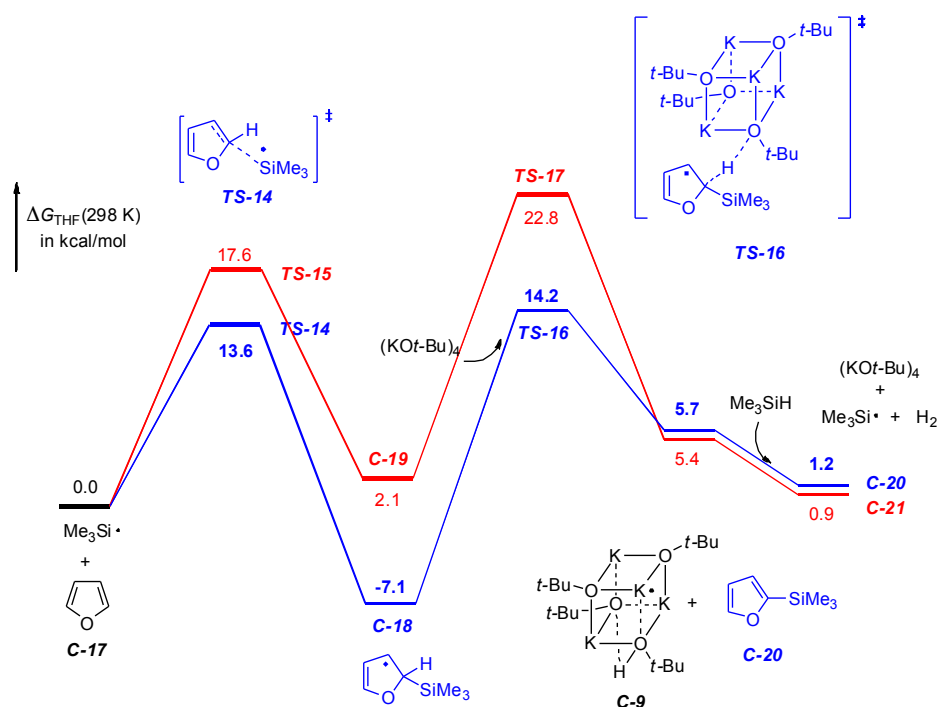
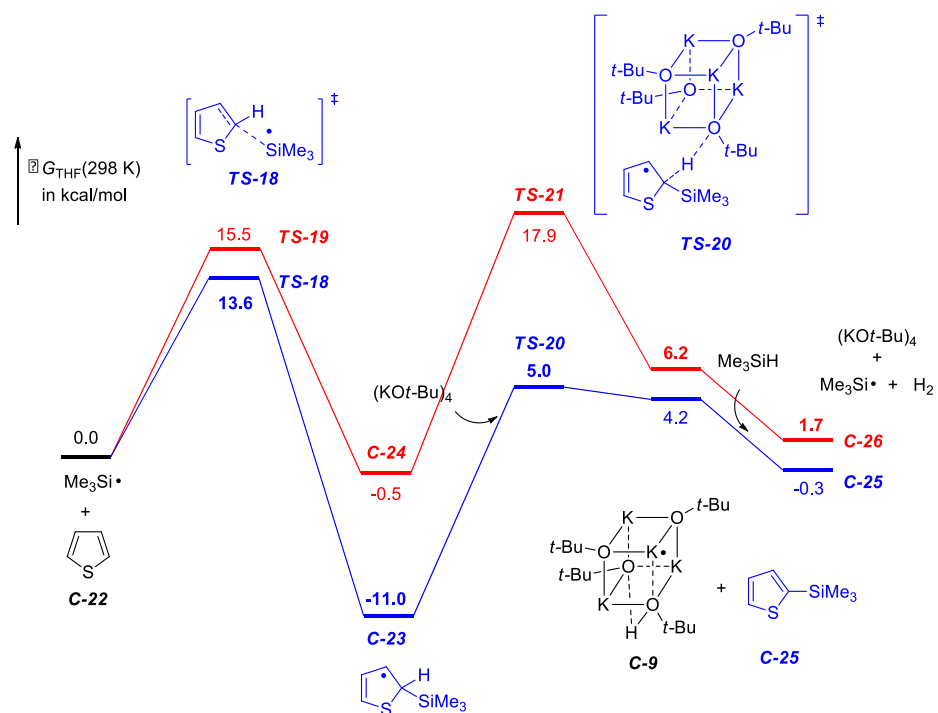


Figure S4.

Free energy profile for C-H silylation of 1-methylpyrrole at C2 and C3 positions. Hydrogen atom is abstracted by tetrameric $(KOt-Bu)_4$. Gibbs free energies, including THF solvation, are shown in kcal/mol.

**Figure S5.**

Free energy profile for C-H silylation of furan at C2 and C3 positions. Hydrogen atom is abstracted by tetrameric $(\text{KOt-Bu})_4$. Gibbs free energies, including THF solvation, are shown in kcal/mol.

**Figure S6.**

Free energy profile for C–H silylation of thiophene at C2 and C3 positions. Hydrogen atom is abstracted by tetrameric (KOt-Bu)₄. Gibbs free energies, including THF solvation, are shown in kcal/mol.

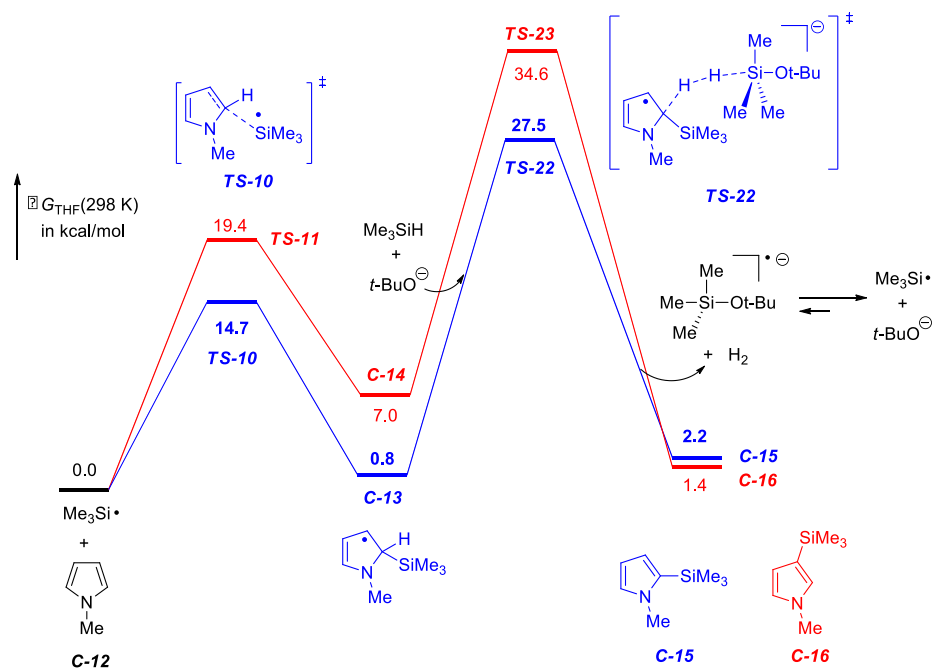


Figure S7.

Free energy profile for C–H silylation of 1-methylpyrrole at C2 and C3 positions. Hydrogen atom is abstracted by pentacoordinate silicate anion. Gibbs free energies, including THF solvation, are shown in kcal/mol.

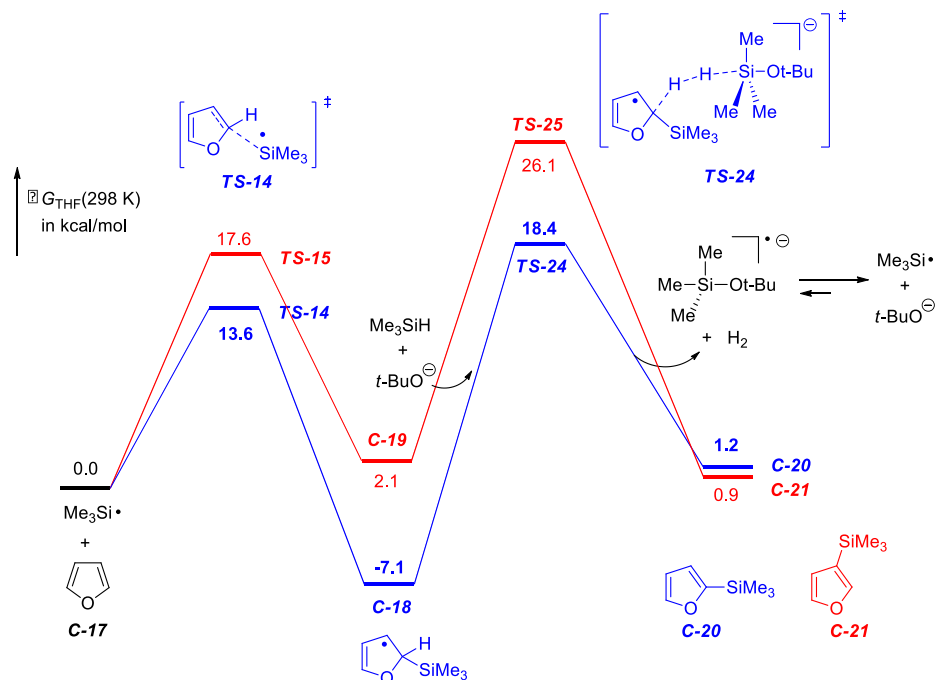


Figure S8.

Free energy profile for C-H silylation of furan at C2 and C3 positions. Hydrogen atom is abstracted by pentacoordinate silicate anion. Gibbs free energies, including THF solvation, are shown in kcal/mol.

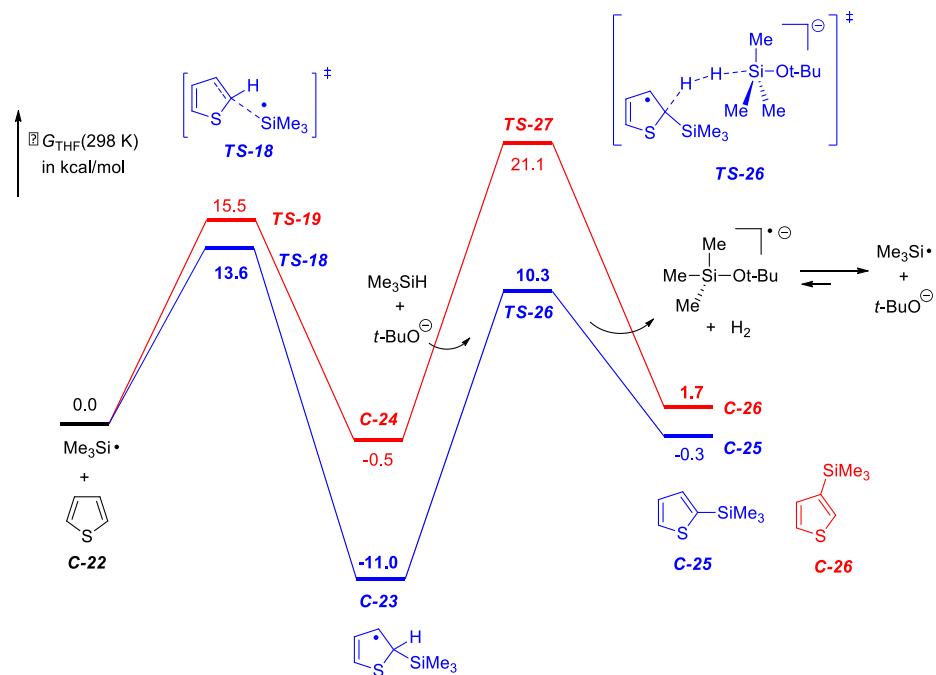


Figure S9.

Free energy profile for C–H silylation of furan at C2 and C3 positions. Hydrogen atom is abstracted by pentacoordinate silicate anion. Gibbs free energies, including THF solvation, are shown in kcal/mol.

^1H NMR concentration dependence of silylation product 2 in CDCl_3 .

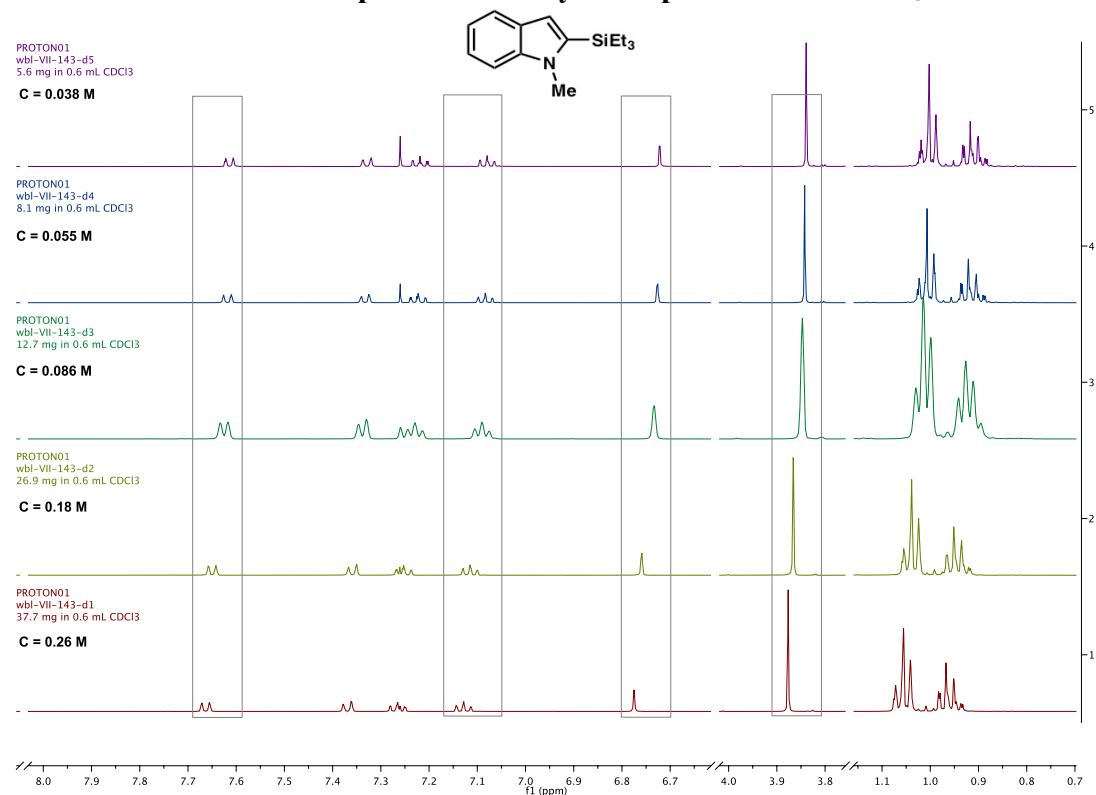
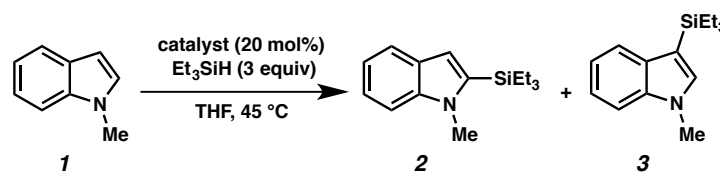


Figure S10

Isolated 1-Methyl-2-(triethylsilyl)-1H-indole was dissolved in CDCl_3 at the indicated concentration and ^1H NMR spectra were acquired, as shown in Figure S10. This demonstrated the anticipated variation for the product signal under reaction or analytical conditions.

General method for the screening of base catalysts and kinetic profile:

entry	catalyst	time (h)	conv (%)	2 : 3
1	KOt-Bu	10	88	11:1
2	KOEt	10	55	9:1
3	KOMe	20	35	9:1
4	KOTMS	20	53	12:1
5	KOAc	60	0	–
6	KOH	20	52	11:1
7	KH	36	0	–
8	KC ₈	10	73	8:1
9	CsOH·H ₂ O	10	64	8:1
10	RbOH·xH ₂ O	10	38	10:1
11	LiOt-Bu	36	0	–
12	NaOt-Bu	36	0	–
13	Mg(Ot-Bu) ₂	36	0	–
14	Ca(Oi-Pr) ₂	36	0	–
15	Ba(Ot-Bu) ₂	36	0	–
16	Al(Ot-Bu) ₃	36	0	–

Table 1

In a nitrogen-filled glove box, 1-methylindole (0.5 mmol, 1 equiv), triethylsilane (1.5 mmol, 3 equiv), the indicated base (0.1 mmol, 20 mol%), and THF (5 mL) were added to a 1 dram vial equipped with a magnetic stirring bar. At the indicated time, aliquots were removed using a glass capillary tube, diluted with Et₂O, and analyzed using GC-FID to determine regioselectivity and yield. GC conversion is reported as product (C2- and C3-silylation) divided by product and starting material. For further base screening, see the Supporting Information of our initial disclosure.⁹

Procedure for time course reaction monitoring by in situ ¹H NMR

In a nitrogen-filled glove box, a stock solution containing KOt-Bu (60.5 mg, 0.539 mmol) and 1,2,5-trimethoxybenzene (if used, 45.4mg, 0.267 mmol) is prepared in THF-D₈ (2.7 ml). Continuing in the glove box, a J-Young gas-tight NMR tube is then charged

⁹ Toutov, A. A.; Liu, W.-B.; Betz, K. N.; Fedorov, A.; Stoltz, B. M.; Grubbs, R. H. *Nature* **2015**, 518, 80–84

with 1-methylindole (32.8 mg, 0.25 mmol, 1 equiv), Et₃SiH (0.75 mmol, 3 equiv), and 0.25 mL of stock solution. The tube is tightly capped with the corresponding Teflon plug, removed from the glove box, placed in the bore of the NMR, and heated to 45 °C. ¹H NMR spectra were acquired in “array” mode, with a spectrum taken approximately every 3 minutes for the length of experiment. The data was processed using MestReNova and peak integrations were normalized to 1,2,5-trimethoxybenzene (if used). Data is displayed using the MestReNova “stack” function with the axis to the right corresponding to NMR scan number, Scheme 3.

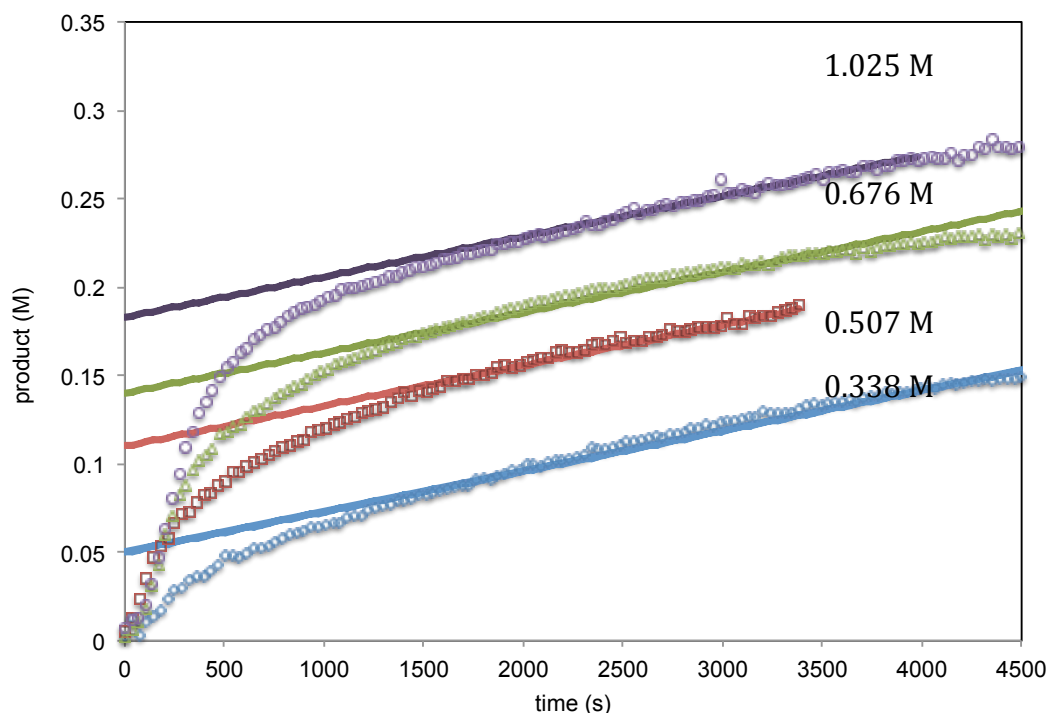


Figure S11

A study was conducted following the procedure for time course reaction monitoring by ¹H NMR (using internal standard) while varying indole [**1**], from 0.25–0.76 mmol (0.5–1.5 equiv). We observed an initial burst phase of product formation, unfortunately due to the induction period we had difficulty assigning an initial rate for this phase but all trials appear to have a similar rate during the burst phase. The length of the burst phase (i.e. product formed) appears to be related to indole [**1**]. Interestingly, after the burst phase the slope of all 4 plots appear to be consistent, indicating the reaction may not depend on [**1**]. This work helped us to understand the reaction occurred in the following 3 regimes;

induction, burst, and sustained reaction periods. *Note: induction period was deducted for each experiment.*

Procedure for time course reaction monitoring by GC analysis of reaction aliquots

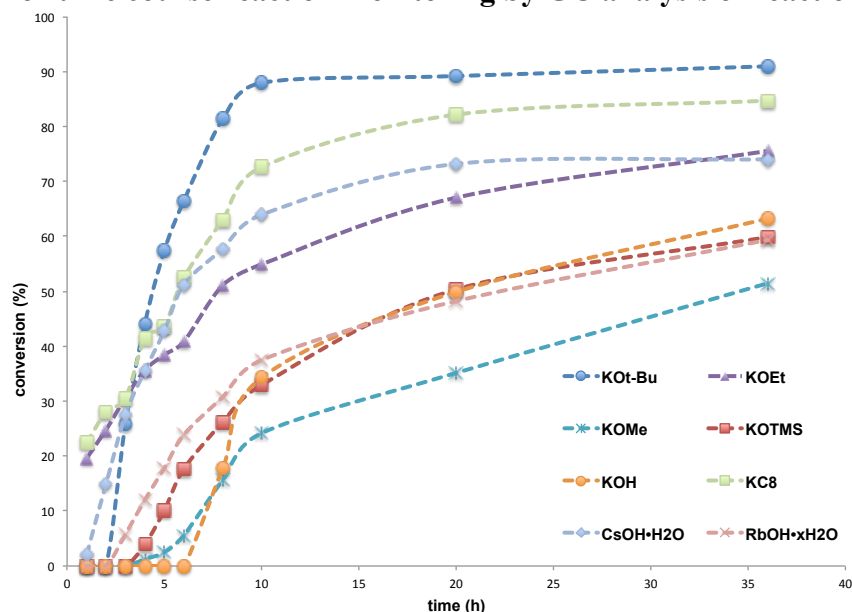


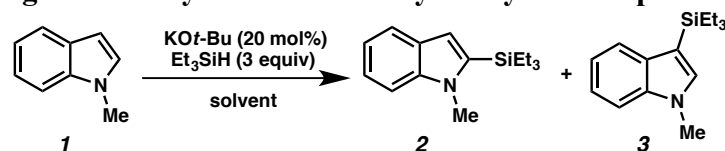
Figure 2

In a nitrogen-filled glove box, 1 dram vials with magnetic stirring bars were charged with the indicated base (0.1 mmol, 20 mol%, as noted in Figure 2, RbOH supplied as unknown hydrate from Strem and used as received), 1-methylindole (65.6 mg, 0.5 mmol, 1 equiv), triethylsilane (174.4 mg, 1.5 mmol, 3 equiv) and THF (0.5 mL, 1M) then sealed with a PTFE-lined screw-cap and heated to 45 °C while stirring. At the indicated time points, an aliquot was removed with a clean, dry glass capillary tube, diluted with Et₂O, and analyzed by GC-FID. Conversion is reported as the percent of both C2- and C3-silylation products divided by products and starting material. Regioselectivity (i.e. C2- to C3-silylation ratios, Table S1) were also obtained at each time point.

Base	Time (h)	Conversion	C2:C3 ratio (x:1)	Base	Time (h)	Conversion	C2:C3 ratio (x:1)	Base	Time (h)	Conversion	C2:C3 ratio (x:1)
KOt-Bu	1.0	0.0	-	KOEt	1.0	19.7	-	CsOH	1.0	2.2	>20
	2.0	0.0	-		2.0	24.8	26.8		2.0	14.9	21.4
	3.0	25.8	27.3		3.0	30.6	22.3		3.0	27.6	23.0
	4.0	44.2	24.1		4.0	35.7	19.4		4.0	35.6	20.5
	5.0	57.4	23.2		5.0	38.5	19.2		5.0	42.8	19.5
	6.0	66.5	12.8		6.0	40.9	11.4		6.0	51.2	12.1
	8.0	81.4	16.9		8.0	51.1	14.0		8.0	57.7	15.2
	10.0	88.0	15.0		10.0	54.9	12.5		10.0	64.0	11.6
	20.0	89.2	15.0		20.0	67.1	8.2		20.0	73.2	7.7
	36.0	91.0	9.3		36.0	75.6	6.2		36.0	74.0	5.8
KOTMS	1.0	0.0	-	KOMe	1.0	0.0	-	RbOH	1.0	0.0	-
	2.0	0.0	-		2.0	0.0	-		2.0	0.0	-
	3.0	0.0	-		3.0	0.0	-		3.0	5.8	5.3
	4.0	3.9	7.1		4.0	1.2	>20		4.0	12.1	10.5
	5.0	10.2	9.9		5.0	2.5	>20		5.0	17.8	18.9
	6.0	17.7	9.0		6.0	5.6	7.0		6.0	23.9	19.9
	8.0	26.2	19.9		8.0	15.7	15.4		8.0	30.8	14.1
	10.0	33.0	14.1		10.0	24.2	12.3		10.0	37.5	11.0
	20.0	50.4	11.6		20.0	35.2	14.9		20.0	48.2	9.5
	36.0	59.9	9.0		36.0	51.5	7.2		36.0	59.4	7.9
KHMDS	1.0	0.0	-	KOH	1.0	0.0	-	KC8	1.0	22.4	>20
	2.0	0.0	-		2.0	0.0	-		2.0	28.0	33.1
	3.0	0.0	-		3.0	0.0	-		3.0	30.6	23.1
	4.0	1.2	>20		4.0	0.0	-		4.0	41.4	21.2
	5.0	2.5	>20		5.0	0.0	-		5.0	43.7	22.8
	6.0	4.7	9.7		6.0	0.0	-		6.0	52.5	14.6
	8.0	8.3	15.0		8.0	17.8	>20		8.0	63.0	14.9
	10.0	10.3	11.0		10.0	34.3	18.4		10.0	72.6	8.5
	20.0	21.6	21.5		20.0	49.9	11.3		20.0	82.2	7.7
	36.0	34.9	7.3		36.0	63.2	7.0		36.0	84.7	5.0

Table S1

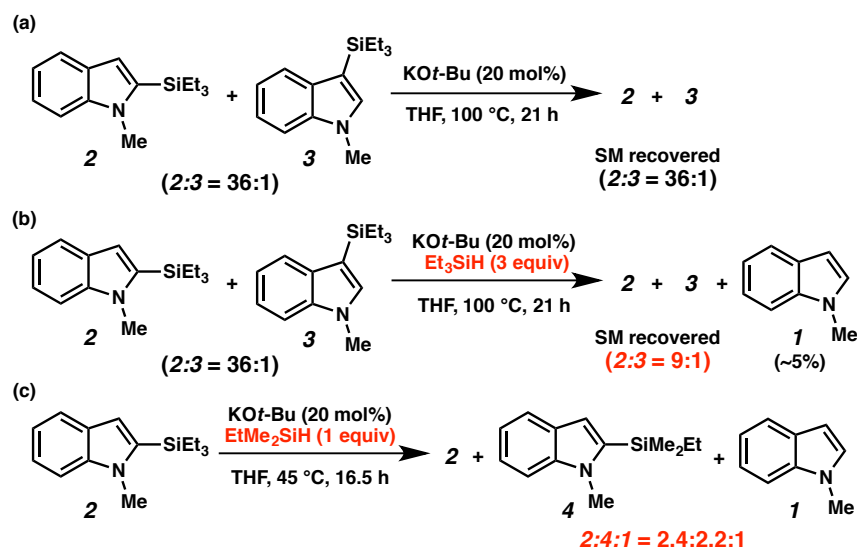
Procedure for regioselectivity and reversibility of silylation experimentation



entry	solvent	temp (°C)	time (h)	conv (%) ^b	2:3 ^b
1	THF	45	10	88	11:1
2	THF	45	15d ^c	>95	1:>20
3	THF	100	20	94	1:9
4	neat	45	48	88	>20:1
5	neat	100	24	>95	4:1

Table 2

In a nitrogen-filled glove box, 1 dram vials were charged with KOt-Bu (0.1 mmol, 20 mol), 1-methylindole (65.6 mg, 0.5 mmol, 1 equiv), triethylsilane (174.4 mg, 1.5mmol, 3 equiv) and THF if used (0.5 mL, 1M) then sealed with a PTFE-lined screw-cap and heated to the indicated temperature. After the indicated reaction time, the crude reaction mixture was diluted with Et₂O, or a small aliquot was removed by glass capillary tube, and analyzed by GC-FID.



Scheme 2

Reversibility (a, b)

In a nitrogen-filled glove box, 1 dram vials with a magnetic stir bar were charged with a mixture of **2** and **3** (24.2 mg, 0.1 mmol, 1 equiv, ratio of **2:3** determined by GC-FID), KOt-Bu (2.4 mg, 0.02 mmol, 20 mol%), Et₃Si-H (49 μ L, 3 mmol, 3 equiv), and THF (0.1 mL, 1 M). The reactions were heated to 100 °C and stirred for the indicated time, after which they were quenched with Et₂O and analyzed by GC (See general method for KOt-Bu-catalyzed silylation for further details).

Cross-over experiment (c)

In a nitrogen-filled glove box, 1 dram vials with a magnetic stir bar were charged with **2** (122.7 mg, 0.5 mmol, 1 equiv), KOt-Bu (11.2 mg, 0.1 mmol, 20 mol%), EtMe₂Si-H (44 mg, 0.5 mmol, 1 equiv), and THF (0.5 mL, 1 M). The reaction was heated to 45 °C and stirred for the indicated time, then quenched with Et₂O (ca. 1mL), concentrated in vacuo, and analyzed by ¹H NMR. Product ratio assigned by correlation to known products.⁹ Note, product ratio of **2** : **3** outside of ¹H NMR detection.

General procedure of gas collection by eudiometry:

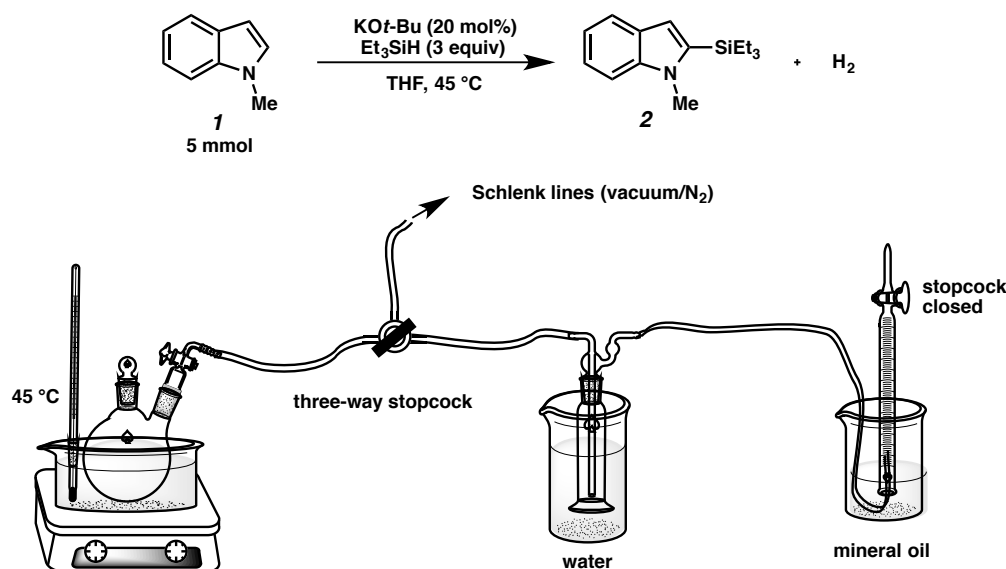


Figure S12.

The eudiometer apparatus used for measuring H₂ gas evolution in the KO^{*t*}-Bu-catalyzed cross-dehydrogenative silylation reactions. Note that a Schlenk round-bottom flask with a Teflon valve was used instead of the two neck round bottom flask and ground glass stopcock as depicted above.

In a nitrogen-filled glove box, KO^{*t*}-Bu (114 mg, 1 mmol, 20 mol%), 1-methylindole (656.4 mmol, 1 equiv), and THF (5 mL) were added to a 25 mL Schlenk flask equipped with a magnetic stirring bar, followed by silane (2.4 mL, 15 mmol, 3 equiv). The flask was sealed and removed from the glove box and placed in a preheated oil bath (45 °C). After stirring at 800 rpm for 15 min for equilibration, the side neck of the Schlenk flask was quickly connected to the gas collection set up (see figure S12). The reactions was stirred for another 20 min (at which point the apparatus was set to volume = 0 mL), the gas volume was recorded over 4 h. For experiment 1, 80 mL of H₂ gas was collected, and the conversion by ¹H NMR based on silylation product **2** was 72%. For experiment 2: 77 mL of H₂ gas was collected, and the conversion by ¹H NMR based on silylation product **2** was 73%. The gas was confirmed by ¹H NMR as H₂ by transferring to a J-Young gas-tight NMR tube with 0.6 mL of liquid N₂ froze C₆D₆. A control experiment with Et₃SiH (2.4 mL) in THF (5 mL) heated to 45 °C in the identical reaction setup resulted in no gas formation in 10 h.

Procedure for silylation reaction in the presence of TEMPO.

Variation from general conditions

None		3 mol% TEMPO at T= 0 h	
Time (h)	Conversion (%)	Time (h)	Conversion (%)
0.5	0	0.5	0
1	0	1	0
2	2.442617647	2	0
3.33	50.25161871	3.33	0
3.8	70.40868887	3.8	0
4.3	72.5908058	4.3	0.908256973
5.5	89.3022064	4.8	20.18297787
6	92.55487299	5.5	49.71398931
7	92.6937744	6	62.92026299
8	94.73007069	7	76.35299445
11	95.84683421	8	84.92338978
24	95.92848947	11	89.76274718

3 mol% TEMPO at T= 3.3 h		6 mol% TEMPO at T= 3.3 h	
Time (h)	Conversion (%)	Time (h)	Conversion (%)
0.5	0	0.5	0
1	0	1	0
2	6.324916305	2	8.125087104
3.33	51.71900754	3.33	52.51216509
3.8	53.42804928	3.8	54.35414073
4.3	56.23763563	4.3	50.48788256
4.8	53.77412828	4.8	55.29061103
5.5	53.19812793	5.5	52.85443624
6	54.00564947	6	55.76279292
7	56.11867427	7	53.77412828
8	71.13455862	8	54.70409148
11	87.73180662	11	63.30704973
		24	88.06746336

Table S2

General Conditions

In a nitrogen-filled glove box, 1 dram vials with magnetic stirring bars were charged with the K_{OT}-Bu (0.1 mmol, 20 mol%), 1-methylindole (65.6 mg, 0.5 mmol, 1 equiv), triethylsilane (174.4 mg, 1.5mmol, 3 equiv), 2,2,6,6-Tetramethyl-1-piperidinyloxy (TEMPO, 3 or 6 mol% if used), and THF (0.5 mL, 1M) then sealed with a PTFE-lined screw-cap and heated to 45 °C while stirring. At the indicated time points, an aliquot was removed with a clean, dry glass capillary tube, diluted with Et₂O, and analyzed by GC-FID. Conversion is reported as the percent of both C2- and C3-silylation products

divided by products and starting material. Despite our efforts, we were not able to observe the TEMPO–SiEt₃ adduct by GC-MS from above experiments.

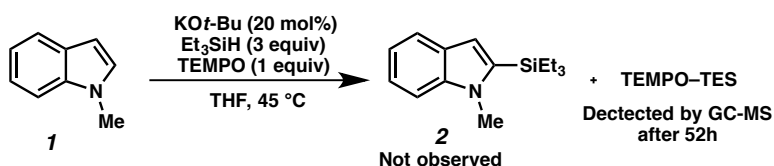


Figure S13

Following the general procedure above, but using 1 equiv of TEMPO resulted in no product formation. After 52 h the TEMPO–SiEt₃ (TEMPO–TES) adduct was observed by GC-MS and after 91 h the ratio of TEMPO:TEMPO–TES was 40:60. A control experiment conducted in the exact same manner but excluding indole **1** (i.e. TEMPO, KO*t*-Bu, Et₃SiH, and THF) also resulted in the detection of TEMPO–TES after 52 h. At 91 h, the ratio of TEMPO:TEMPO–TES was 34:66. No TEMPO adduct was observed when NaO*t*-Bu was in this same control reaction after 9 days.

Effect of additives on the silylation reaction

entry	additive	amount (mol%)	time (h)	conversion (%)	2:3
1	1,10-phenanthroline	5	8 24	52 79	>20:1 >20:1
2	N-methylpyrrolidone	5	8 24	0 50	— >20:1
3	N-methylglycine	5	8 24	7 67	>20:1 19:1
4	glycine	5	8 24	10 54	>20:1 >20:1
5	none	5	8	93	>20:1
6	H ₂ O	10	10 21	6.7 48	>20:1 >20:1
7	H ₂ O	20	10 21	9.8 40	>20:1 >20:1
8	H ₂ O	50	10 21	1 9.2	— >20:1
9	H ₂ O	100	10 21 72	0 0 2.5	—
6	<i>t</i> -BuOH	10	10 21	2 55	>20:1 >20:1
7	<i>t</i> -BuOH	20	10 21	3 42	>20:1 >20:1
8	<i>t</i> -BuOH	50	10 21 72	3 3 4	—
9	<i>t</i> -BuOH	100	10 21 72	3 3 4	—

Table S3

1 dram vials with magnetic stirring bars were charged with the KO*t*-Bu (0.1 mmol, 20 mol%), 1-methylindole (65.6 mg, 0.5 mmol, 1 equiv), triethylsilane (174.4 mg, 1.5 mmol, 3 equiv), additive, and THF (0.5 mL, 1M) then sealed with a PTFE-lined screw-cap and heated to 45 °C while stirring. At the indicated time points, an aliquot was removed with a clean, dry glass capillary tube, diluted with Et₂O, and analyzed by GC-FID. Conversion is reported as the percent of both C2- and C3-silylation products divided by products and starting material. All additives increased the length of the induction period and result in lower yields overall. For the impact additional additives have on the silylation of benzothiophene, see the Supplementary Information of our initial disclosure.⁹

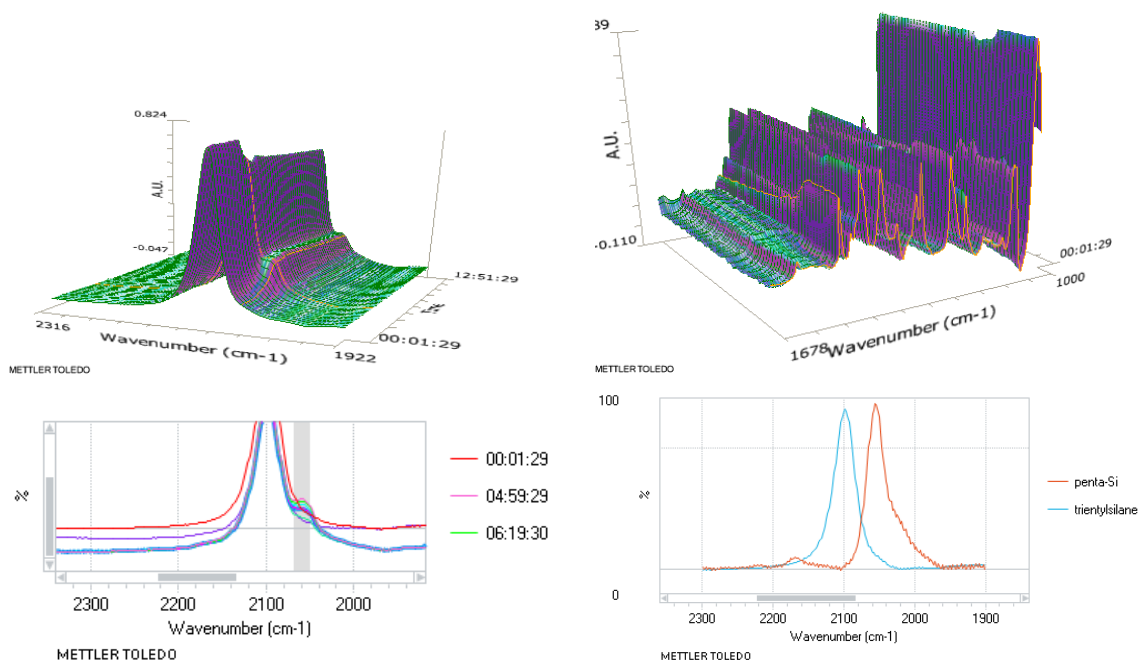
Procedure for reactions using chemical generation of *tert*-butoxyl radical

entry	conditions	mol%	temp (°C)	time (h)	conv (%)	detection of 5
1	KOt-Bu	20	45	24	80	yes
2	DTBP	20	135	14	1	no
3	DTBP	100	135	14	10	no
4	DTBP + KOt-Bu	20, 20	45	14	42	yes
5	TBHN	10	45	10 24	0 0	no no
6	TBHN + NaOt-Bu	10, 20	45	10 24	0 0	no no
7	TBHN + KOt-Bu	10, 20	45	10 24	0 54	no yes

Table 4

Note-sufficient precautions should be taken with all peroxide reagents.

In a nitrogen-filled glove box, 1 dram vials with magnetic stirring bars were charged with peroxide source [*t*-BuO–O*t*-Bu (DTBP) or *t*-BuO–N=N–O*t*-Bu (TBHN)], KO*t*-Bu (if used, 0.1 mmol, 20 mol%), 1-methylindole (65.6 mg, 0.5 mmol, 1 equiv), triethylsilane (174.4 mg, 1.5 mmol, 3 equiv), and THF (0.5 mL, 1M) then sealed with a PTFE-lined screw-cap, and heated indicated temperature while stirring (heating at 135 °C conducted in a fume hood outside of the glove box). At the indicated time points, an aliquot was removed with a clean, dry glass capillary tube, diluted with Et₂O, and analyzed by GC-MS. A number of unidentified impurities were produced along with 10% **2** in entry 3.

Procedure for reaction time course using ReactIR.**Figure S14**

A representative ReactIR spectrum showing the growth of the new Si–H peak assigned to the pentacoordinate species, followed by injection of substrate and immediate product formation. Time axis is shown in the format “hh:mm:ss”.

The glass reaction vessel for use with the ReactIR Sentinel high-pressure probe and a magnetic stirring bar were oven dried, fitted with the PTFE adapter, and brought into a nitrogen-filled glove box, or cooled under a flow of argon and standard air-free technique is used for all additions. *KOt*-Bu (0.8 mmol, 20 mol%), 1-methylindole (1.05 g, 8 mmol, 1 equiv), triethylsilane (13.89 mL, 24 mmol, 3 equiv), additive, and THF (8 mL, 1M) were added to reaction vessel, which was fitted to the ReactIR probe and heated to 45 °C while stirring under argon. The spectrum was recorded over the course of the reaction and data was analyzed using the ReactIR software.

An analogous experiment was performed whereby the indole **1** is not added until the new peak attributed to the pentacoordinate silicate is seen. Indole **1** is then added via syringe and the reaction immediately proceeds with no induction period.

General procedure of ATR-FTIR measurement:

$\text{MOR} + \text{Et}_3\text{Si-X (5 equiv)} \xrightarrow[\text{t (h)}]{\text{THF, 45 } ^\circ\text{C}}$
 $\left[\begin{array}{c} \text{H} \\ | \\ \text{Et}-\text{Si}^+-\text{Et} \\ | \\ \text{OR} \end{array} \right] \text{M}^\oplus \text{XX}^-$
 $\xrightarrow[\text{(Et}_3\text{SiH and THF removal)}]{\text{volatiles evaporation}}$
IR spectra measurement

entry	Base	[Si]-X	t (h) ^a	ν [Si-H] (cm ⁻¹) ^b	$\Delta\nu$ (cm ⁻¹) ^c
1	–	Et ₃ SiH	–	2099	–
2	KOt-Bu	Et ₃ SiH	2	2028	71
3	KOEt	Et ₃ SiH	2	2016	83
4	KOMe	Et ₃ SiH	7	2054	45
5	KOTMS	Et ₃ SiH	7	2047	52
6	KOH	Et ₃ SiH	20	2045	54
7	RbOH·xH ₂ O	Et ₃ SiH	7	2052	47
8	CsOH·H ₂ O	Et ₃ SiH	7	2051	48
9	NaOt-Bu	Et ₃ SiH	36	–	–
10	KOt-Bu	Et ₃ SiD	12	–	–
11	KOt-Bu	Et ₃ SiH (2.5 equiv) + Et ₃ SiD (2.5 equiv)	12	2029	70
12	Mg(Ot-Bu) ₂	Et ₃ SiH	36	–	–
13	LiOt-Bu	Et ₃ SiH	36	–	–

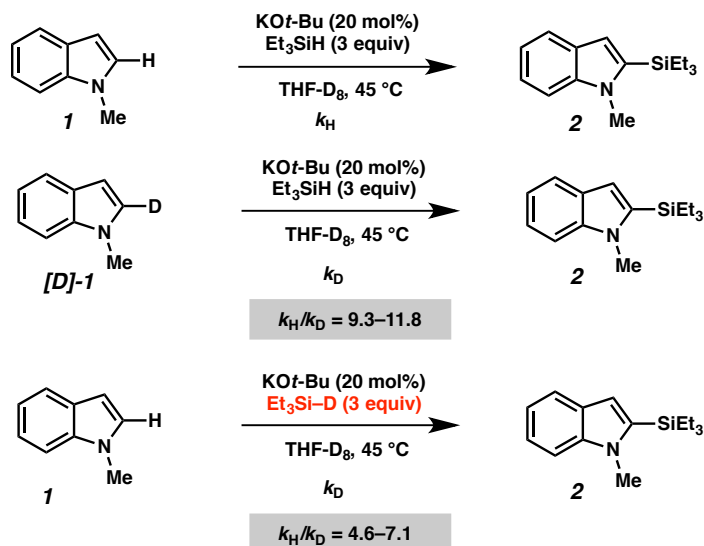
Table S4

^aThe mixture was stirred for the indicated time before IR spectrum was measured. ^bFrequency of Si–H bond stretching. ^cFrequency shift of observed pentacoordinated species from Et₃Si–H.

In a nitrogen-filled glove box, base (0.1 mmol), Et₃SiH (80 μ L, 0.5 mmol, 5 equiv), and THF (0.5 mL) were added to a 1 dram scintillation vial equipped with a magnetic stirring bar. The vial was sealed and the mixture stirred at 45 $^\circ$ C for the indicated time as shown in Table S4. The vial was transferred to another nitrogen-filled glove box with an ATR-FTIR and a few drops of this mixture placed on the ATR crystal. After waiting for 5 minutes to evaporate all the volatiles (i.e. THF and silanes), the IR spectrum of the residue was recorded. No new Si–H stretch was observed with bases which did not catalyze the silylation reaction (e.g. NaOt-Bu, Mg(Ot-Bu)₂, or LiOt-Bu) as these did not form the requisite pentacoordinate complex.

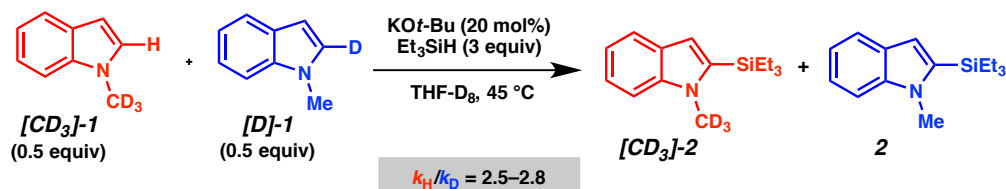
Procedure for kinetic isotope effect

Parallel reactions:



Scheme 5a

The general procedure for reaction monitoring by ^1H NMR was used, with 1,2,5-trimethoxybenzene as the internal standard. A KIE value was obtained using the initial rates method, each experiment was conducted in duplicate.



Scheme 5b

The general procedure for reaction monitoring by ^1H NMR was used, without the use of internal standard and using 0.5 equiv of both $[CD_3]-1$ and $[D]-1$. The KIE value was obtained using the initial rate of product ($[CD_3]-2$ or 2) formation, as these reactions were reversible and reached comparable product yields at later time points. The experiment was conducted in duplicate.

Procedure for the acquisition of electron paramagnetic resonance (EPR) spectra.

In a nitrogen-filled glove box, KOt-Bu (11.2 mg, 0.1 mmol), Et₃SiH (81 μL , 0.5 mmol, 5 equiv), and THF (0.5 mL) were added to a 1 dram scintillation vial equipped with a magnetic stirring bar. The vial was sealed and the mixture stirred at 45 $^\circ\text{C}$ for 5 h. The

reaction mixture was then transferred into an EPR tube, fitted with a plastic cap, taped with parafilm, removed from the glove box, and quickly frozen in liquid nitrogen. The sample was kept at 77 °K and the EPR spectrum was acquired at 77 °K. A signal at approximately $g=2.007$ was observed, further investigations to identify radical intermediates spectroscopically is currently an active area of this project (see page S52 for the spectrum).

Procedure for reaction calorimetry

A number of experiments were conducted to probe the thermodynamics of the silylation reaction. We observed no detectable heatflow during these experiments. We previously had concerns relating to the scalability of the silylation reaction, given the rapid formation of product, but were pleased to find reaction exotherm should not be an issue.

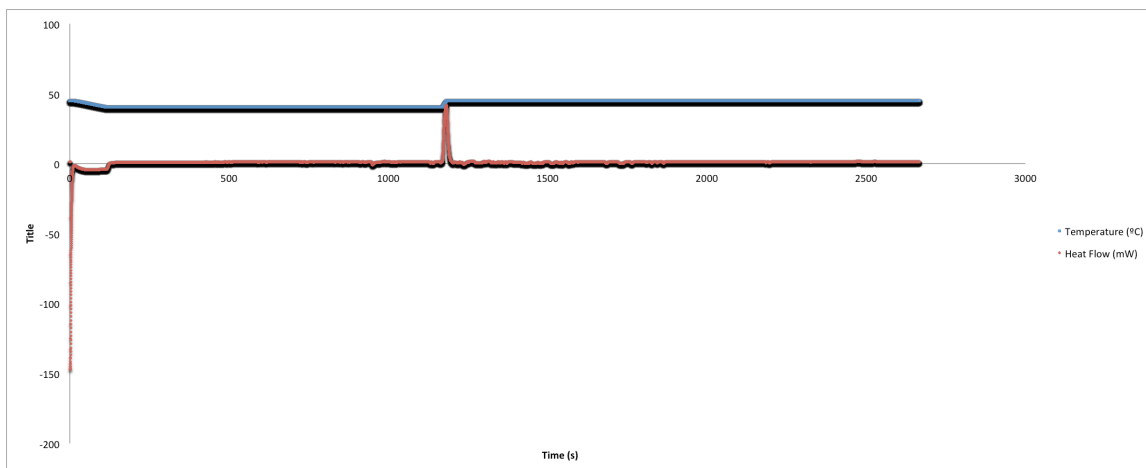


Figure S15

A calorimeter screw cap vial is flame dried and cooled in a vacuum desiccator with the corresponding cap and septum. $\text{KO}t\text{-Bu}$ (112.2 mg, 1 mmol, 20 mol%) is quickly weighed into the vial, which is then evacuated and refilled with argon 3 times. Et_3SiH (2.4 mL, 15 mmol, 3 equiv) and indole **1** (655.8 mg, 5 mmol, 1 equiv) are added using standard air-free technique. The sample was held at 40 °C overnight with no heatflow detected or silylation product **2** detected by GC or TLC. The temperature was then ramped up to 45 °C, a rapid heat flow corresponding to the sample heating was seen but no further heatflow was observed despite the observed of product upon workup.

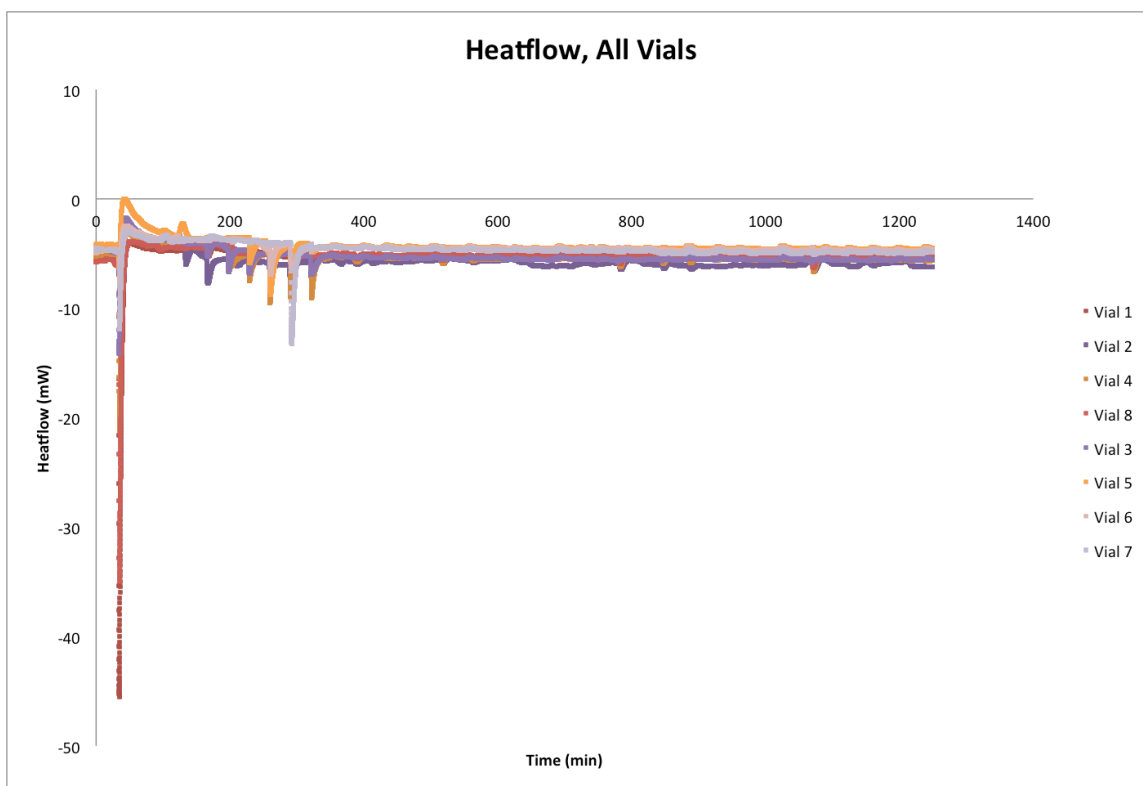


Figure S16

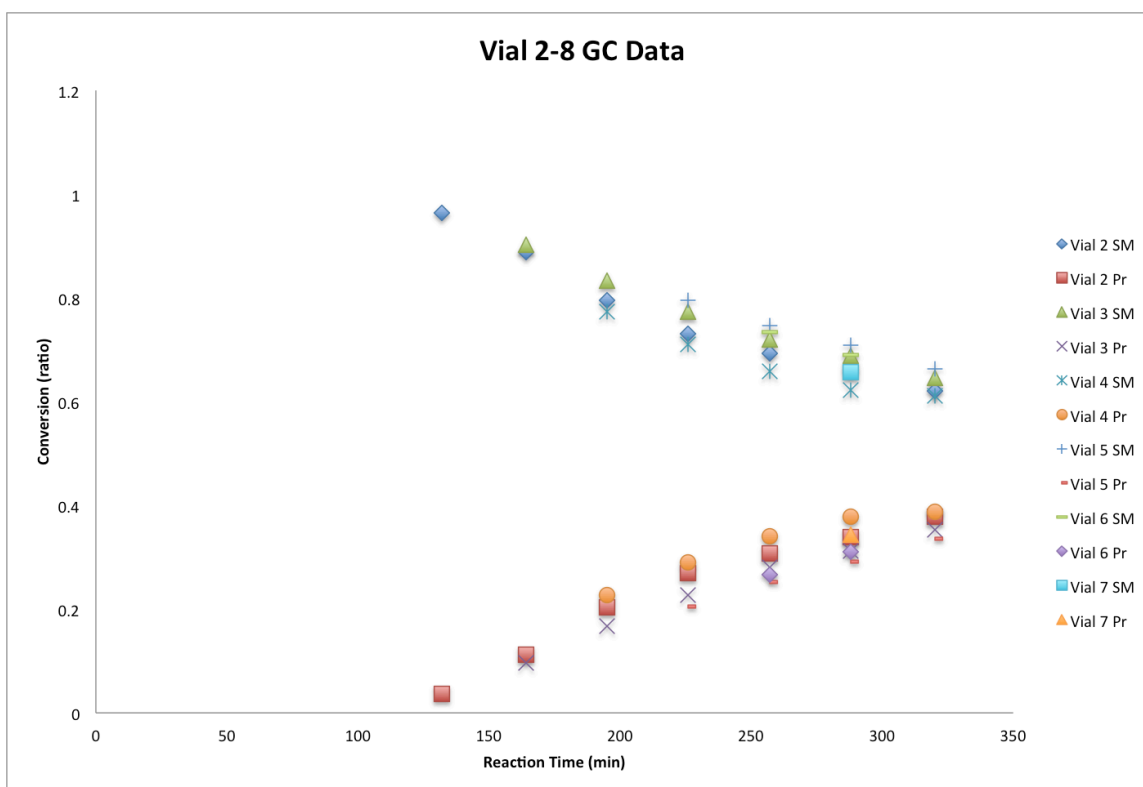
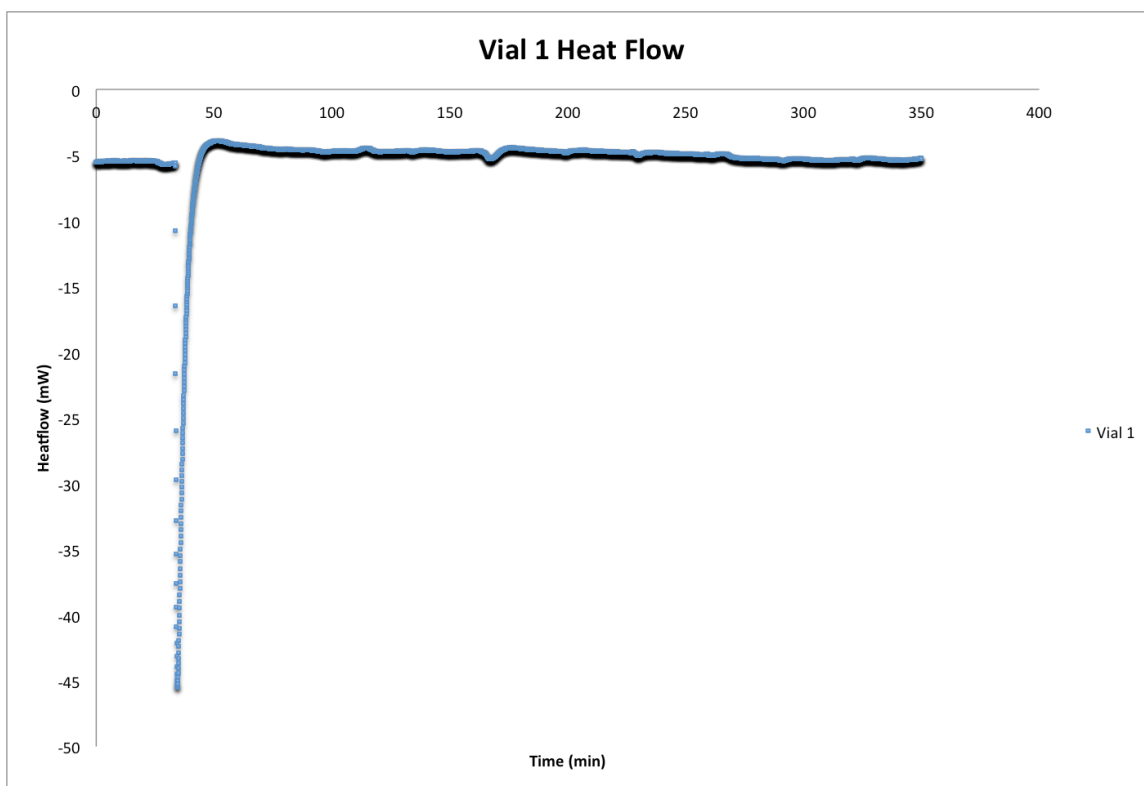
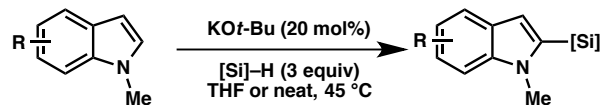


Figure S17

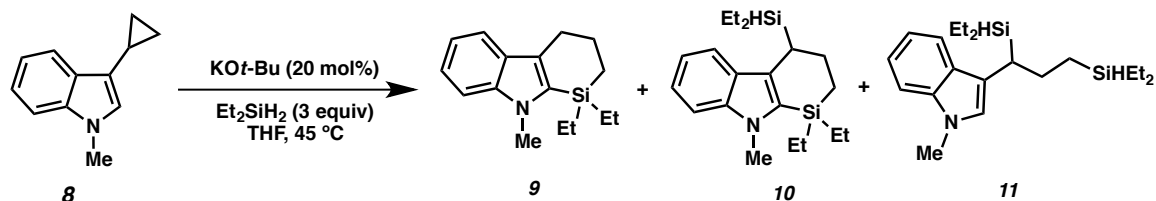
**Figure S18**

A second trial was performed with 8 identical vials in parallel. The calorimeter can detect the temperature change due to minute changes in pressure (i.e. using a syringe and needle to remove an aliquot for a GC sample) as seen in figure S16. Therefore one vial was not sampled until the endpoint (Figure S18), while an additional vial was sampled at each time point (i.e. vial 2 at first time point, then vial 2 and 3 at the second time point, etc.). All vials had comparable conversion upon workup (52–60% C2-silylation product **2**)

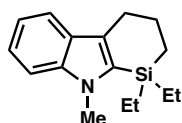
8 calorimeter screw cap vials with the corresponding cap and septum were flame dried and allowed to cool under vacuum, then refilled with argon. Indole **1** (524.7 mg, 4 mmol, 1 equiv), Et₃SiH (1.92 mL, 12 mmol, 3 equiv) and THF (3.2 mL) are added using standard air-free technique. The reactions are equilibrated at 45 °C using an argon filled balloon and then the reaction is initiated using 1M solution of KO^t-Bu (0.8 mL, 0.8 mmol, 20 mol%, equilibrated to 45 °C in plugged syringe). Interestingly, an initial negative heat of mixing is observed. Based on the GC data and variance in the heatflow we observed, we estimate the heat of reaction to be $\pm 1 \text{ kcal}(\text{mol})^{-1}$ or less.

General procedure for KO^t-Bu-catalyzed silylation and characterization data of new compounds.**Figure S19**

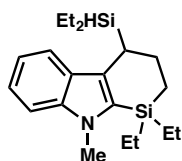
In a nitrogen-filled glove box, KO^t-Bu (11.2 mg, 0.1 mmol, 20 mol%), indole (0.5 mmol, 1 equiv), and THF (0.5 mL, if indicated, see the details below) were added to a 1 dram scintillation vial equipped with a magnetic stirring bar, followed by silane (1.5 mmol, 3 equiv). Then the vial was sealed and the mixture was stirred at 45 °C for the indicated time. The vial was removed from the glove box, diluted with diethyl ether (2 mL) and concentrated under reduced pressure. The regioselectivity (C2 silylation product to C3 silylation product: C2:C3) was determined by ¹H NMR or GC analysis of the crude mixture. The residue was purified by silica gel flash chromatography to give the desired product.

**Figure S20**

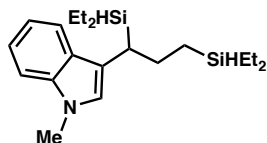
The general procedure was followed. The reaction was performed with KO^t-Bu (6.7 mg, 0.06 mmol, 20 mol%), 3-cyclopropyl-1-methyl-1H-indole **8** (51.3 mg, 0.3 mmol, 1 equiv), Et₂SiH₂ (79.2 mg, 0.9 mmol, 3 equiv), and 0.3 mL of THF at 45 °C for 10 days. Three products shown above, along with some unidentified impurity, were isolated by silica gel flash chromatography (3% CH₂Cl₂ in hexanes). Unreacted starting material **8** was recovered in 30% yield (15.4 mg). Analytic pure compounds **9** (3.9 mg, 5% yield), **10** (8.8 mg, 8% yield), and **11** (1.9 mg, 3% yield) were purified by preparative HPLC (ACE 5 C18, 250 x 21 2mm id column; gradient, 30→80% MeCN in H₂O in 3 min, then 80→100% MeCN in H₂O in 7 min, followed by 100% MeCN; flow rate = 10 mL/min; λ = 230 nm.).



1,1-Diethyl-9-methyl-2,3,4,9-tetrahydro-1H-silino[2,3-b]indole 9: $R_f = 0.5$ (10% CH_2Cl_2 in hexanes); ^1H NMR (400 MHz, CDCl_3) δ 7.55 (dt, $J = 7.9, 1.0$ Hz, 1H), 7.29 (dt, $J = 8.3, 0.9$ Hz, 1H), 7.22 (ddd, $J = 8.2, 6.9, 1.2$ Hz, 1H), 7.07 (ddd, $J = 7.9, 6.8, 1.1$ Hz, 1H), 3.78 (s, 3H), 2.91 – 2.80 (m, 2H), 2.07 – 1.95 (m, 2H), 1.05 – 0.90 (m, 8H), 0.90 – 0.78 (m, 4H); ^{13}C NMR (100 MHz, CDCl_3) δ 139.4, 133.6, 128.3, 127.4, 122.2, 118.8, 118.3, 108.9, 33.1, 25.2, 23.0, 8.9, 7.9, 6.0. IR (Neat Film NaCl) 2951, 2909, 2872, 1504, 1455, 1361, 1336, 1307, 1234, 1165, 1138, 1011, 920, 806, 761 cm^{-1} ; HRMS (FAB+) calc'd for $\text{C}_{16}\text{H}_{23}\text{NSi}$ $[\text{M}]^+$: 257.1600, found: 257.1601.



4-(Diethylsilyl)-1,1-diethyl-9-methyl-2,3,4,9-tetrahydro-1H-silino[2,3-b]indole 10: $R_f = 0.5$ (10% CH_2Cl_2 in hexanes); ^1H NMR (400 MHz, CDCl_3) δ 7.48 (dt, $J = 7.9, 1.0$ Hz, 1H), 7.26 (dt, $J = 8.2, 1.0$ Hz, 1H), 7.19 (ddd, $J = 8.2, 6.8, 1.2$ Hz, 1H), 7.02 (ddd, $J = 7.9, 6.8, 1.1$ Hz, 1H), 3.82 – 3.79 (m, 1H), 3.77 (s, 3H), 2.84 – 2.81 (m, 1H), 2.36 – 2.30 (m, 1H), 2.07 – 1.98 (m, 1H), 1.06 – 0.91 (m, 11H), 0.91 – 0.76 (m, 7H), 0.75 – 0.65 (m, 2H), 0.62 – 0.44 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 139.4, 132.1, 130.0, 127.9, 122.1, 119.5, 117.9, 108.8, 33.1, 25.8, 22.3, 8.63, 8.61, 8.11, 8.09, 7.2, 6.7, 6.1, 3.4, 2.8. IR (Neat Film NaCl) 2953, 2910, 2873, 2100, 1495, 1455, 1414, 1361, 1321, 1262, 1234, 1164, 1135, 1080, 1013, 968, 809, 761 cm^{-1} ; HRMS (FAB+) calc'd for $\text{C}_{20}\text{H}_{33}\text{NSi}_2$ $[\text{M}]^+$: 343.2152, found: 343.2140.



3-(1,3-Bis(diethylsilyl)propyl)-1-methyl-1*H*-indole 11: ^1H NMR (500 MHz, CDCl_3) δ 7.56 (dt, $J = 7.9, 1.0$ Hz, 1H), 7.30 – 7.25 (m, 1H), 7.19 (ddd, $J = 8.2, 6.9, 1.1$ Hz, 1H), 7.06 (ddd, $J = 7.9, 6.9, 1.1$ Hz, 1H), 6.72 (s, 1H), 3.79 – 3.76 (m, 1H), 3.76 (s, 3H), 3.61 (hept, $J = 3.1$ Hz, 1H), 2.46 – 2.34 (m, 1H), 1.97 – 1.77 (m, 2H), 0.98 (t, $J = 7.9$ Hz, 3H), 0.95 – 0.91 (m, 6H), 0.89 (t, $J = 7.9$ Hz, 3H), 0.81 – 0.74 (m, 1H), 0.69 – 0.41 (m, 9H); ^{13}C NMR (125 MHz, CDCl_3) δ 137.0, 128.6, 125.3, 121.3, 119.6, 118.2, 116.4, 109.1, 32.8, 27.0, 25.3, 10.8, 8.6, 8.6, 8.4, 8.4, 2.9, 2.9, 2.4, 2.1. IR (Neat Film NaCl) 2952, 2932, 2910, 2872, 2094, 1469, 1414, 1372, 1325, 2235, 1012, 970, 810, 736 cm^{-1} ; HRMS (FAB+) calc'd for $\text{C}_{20}\text{H}_{35}\text{NSi}_2$ $[\text{M}]^+$: 345.2308, found: 345.2314.

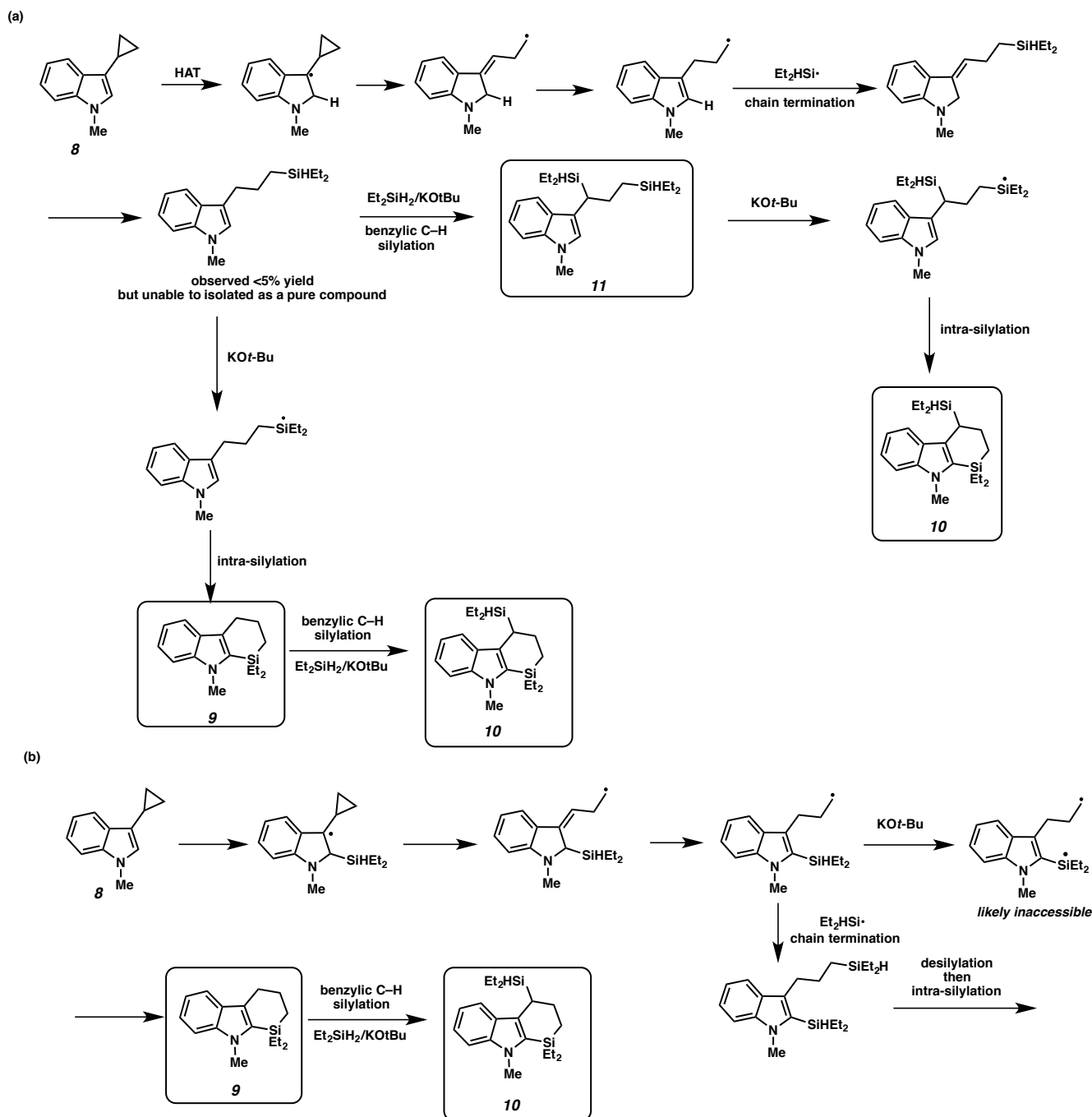
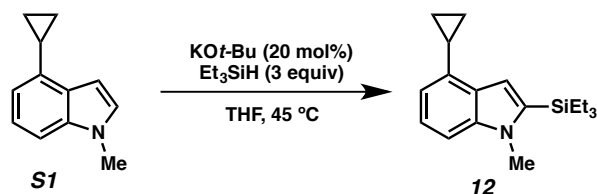
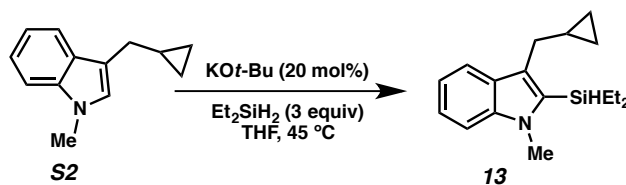
Possible mechanism for the formation of compounds **9**, **10**, **11**

Figure S21 describes a possible route to the formation of **9**, **10**, and **11** through an initial hydrogen atom transfer reaction to substrate **8**. We envision this is possible since the silylation reaction was shown to be reversible, a process which is thought to occur by hydrogen atom transfer (HAT), likely of a pentacoordinate silicate species, to indole **2**.

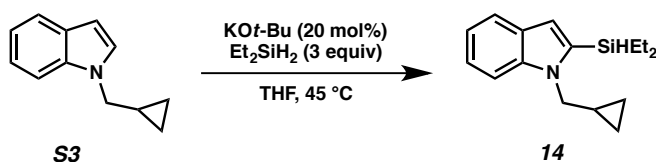
In the case of cyclopropyl-substituted indole **8**, the cyclopropane ring opening is faster than reverse HAT. Figure S21b describes an analogous process but with addition of a silicon radical as compared to a hydrogen radical. The low yield may be explained by a number of radical termination processes limiting reaction rate. A number of these proposed radical intermediates would be high energy and likely to decompose or react in other manners, contributing to the low overall mass balance.



4-cyclopropyl-1-methyl-2-(triethylsilyl)-1H-indol **12:** The general procedure was followed. The reaction was performed with KO*t*-Bu (6.7 mg, 0.06 mmol, 20 mol%), *N*-Methyl-4-(cyclopropyl)-indole **S1** (51.3 mg, 0.3 mmol, 1 equiv), Et₃SiH (146 μ L, 0.9 mmol, 3 equiv), and 0.3 mL of THF at 45 $^\circ$ C for 48 h. The desired product **12** (54.7 mg, 64% yield) was purified by silica gel flash chromatography (5 \rightarrow 10% CH₂Cl₂ in hexanes) as yellow oil. R_f = 0.4 (10% CH₂Cl₂ in hexanes); ¹H NMR (400 MHz, Chloroform-*d*) δ 7.20 – 7.12 (m, 2H), 6.91 (s, 1H), 6.74 – 6.65 (m, 1H), 3.85 (s, 3H), 2.31 (ttd, J = 8.5, 5.2, 0.6 Hz, 1H), 1.10 – 1.01 (m, 11H), 1.00 – 0.92 (m, 6H), 0.91 – 0.86 (m, 2H); ¹³C NMR (101 MHz, Chloroform-*d*) δ 140.05, 137.59, 136.03, 128.59, 122.24, 113.88, 111.28, 106.59, 33.23, 13.06, 8.14, 7.70, 4.16; IR (Neat Film NaCl) 3080, 3051, 3002, 2953, 2909, 2874, 1581, 1503, 1454, 1441, 1415, 1370, 1351, 1323, 1277, 1237, 1171, 1137, 1070, 1017, 977, 885, 841, 787, 769, 745, 734, 700, 679 cm⁻¹; HRMS (MM+) calc'd for C₁₈H₂₇NSi [M+H]⁺: 286.1986 found: 286.1997.



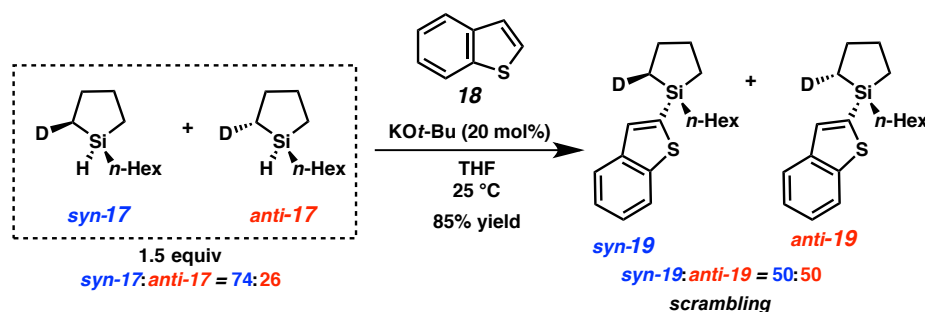
3-(Cyclopropylmethyl)-2-(diethylsilyl)-1-methyl-1H-indole 13: The general procedure was followed. The reaction was performed with KOt-Bu (4.5 mg, 0.04 mmol, 20 mol%), *N*-Methyl-3-(cyclopropylmethyl)-indole **S2** (37.0 mg, 0.2 mmol, 1 equiv), Et₂SiH₂ (78 μ L, 0.6 mmol, 3 equiv), and 0.2 mL of THF at 45 °C for 5 days. The desired product **13** (17.2 mg, 32% yield) was purified by silica gel flash chromatography (2.5% CH₂Cl₂ in hexanes) as colorless oil. R_f = 0.5 (10% CH₂Cl₂ in hexanes); ¹H NMR (500 MHz, CDCl₃) δ 7.67 (dt, J = 7.9, 1.0 Hz, 1H), 7.31 (dt, J = 8.2, 0.9 Hz, 1H), 7.26 (ddd, J = 8.2, 6.8, 1.1 Hz, 1H), 7.10 (ddd, J = 7.9, 6.8, 1.0 Hz, 1H), 4.54 – 4.46 (m, 1H), 3.83 (s, 3H), 2.86 (d, J = 6.4 Hz, 2H), 1.10 – 1.02 (m, 7H), 1.03 – 0.87 (m, 4H), 0.53 – 0.43 (m, 2H), 0.33 – 0.22 (m, 2H); ¹³C NMR (125 MHz, CDCl₃) δ 139.9, 132.3, 128.6, 127.0, 122.3, 119.7, 118.6, 109.1, 32.9, 30.3, 13.3, 8.9, 5.2, 4.8. IR (Neat Film NaCl) 3073, 2999, 2931, 2909, 2872, 2131, 1503, 1457, 1424, 1355, 1319, 1292, 1246, 1228, 1167, 1139, 1087, 1013, 975, 836, 809 cm⁻¹; HRMS (MM+) calc'd for C₁₇H₂₆NSi [M+H]⁺: 272.1829, found: 272.1823.



1-Benzyl-5-methoxy-2-(triethylsilyl)-1H-indole 14: The general procedure was followed. The reaction was performed with KOt-Bu (4.6 mg, 0.04 mmol, 20 mol%), 1-(cyclopropylmethyl)-1H-indole **S3** (34.2 mg, 0.2 mmol, 1 equiv), Et₂SiH₂ (78 μ L, 0.9 mmol, 3 equiv), and 0.2 mL of THF at 45 °C for 96 h. C2:C3 > 20:1. The desired product **14** (29.7 mg, 58% yield) was purified by silica gel flash chromatography (gradient, 2→3.3% CH₂Cl₂ in hexanes) as colorless oil. R_f = 0.5 (10% CH₂Cl₂ in hexanes); ¹H NMR (500 MHz, CDCl₃) δ 7.64 (dt, J = 7.9, 1.0 Hz, 1H), 7.42 (dq, J = 8.3, 0.9 Hz, 1H), 7.26 – 7.18 (m, 1H), 7.10 (ddd, J = 7.9, 6.9, 1.0 Hz, 1H), 6.77 (d, J = 0.9 Hz, 1H), 4.47 (p, J = 3.3 Hz, 1H), 4.17 (d, J = 6.4 Hz, 2H), 1.33 – 1.24 (m, 1H), 1.14 – 1.05

(m, 6H), 1.03 – 0.89 (m, 4H), 0.62 – 0.47 (m, 2H), 0.46 – 0.37 (m, 2H); ^{13}C NMR (126 MHz, CDCl_3) δ 139.6, 136.1, 128.9, 122.0, 120.8, 119.2, 112.8, 110.1, 50.4, 12.3, 8.4, 4.3, 3.8. IR (Neat Film NaCl) 3006, 2955, 2933, 2912, 2874, 2113, 1493, 1466, 1455, 1435, 1413, 1390, 1377, 1351, 1334, 1322, 1301, 1233, 1214, 1165, 1153, 1091, 1047, 1015, 974, 819 cm^{-1} ; HRMS (MM: ESI-APCI+) calc'd for $\text{C}_{16}\text{H}_{24}\text{NSi}$ $[\text{M}+\text{H}]^+$: 258.1673, found: 258.1676.

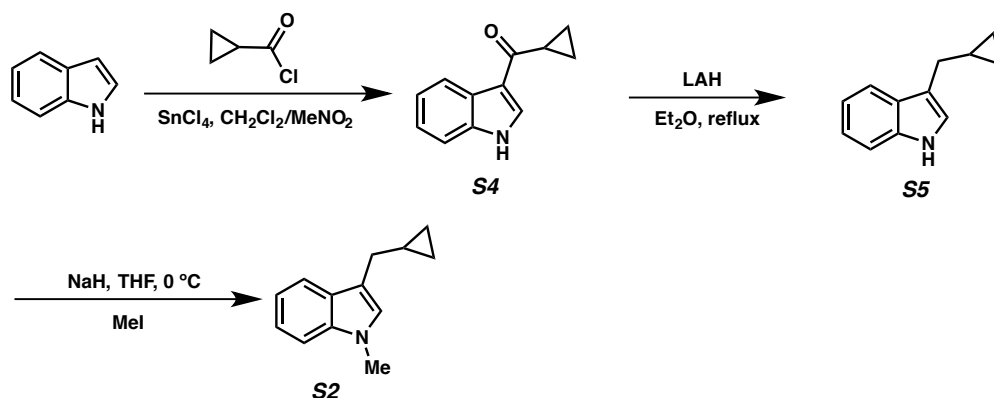
Stereochemical course of the KOt-Bu -catalyzed C–H silylation of benzo[*b*]thiophene.



1-(Benzo[*b*]thiophen-2-yl)-1-hexylsilolane 19: In a nitrogen-filled glove box, KOt-Bu (4.5 mg, 0.04 mmol, 20 mol%) and benzo[*b*]thiophene **18** (26.8 mg, 0.20 mmol, 1.0 equiv) were added to an oven-dried scintillation vial equipped with a magnetic stirring bar, followed by deuterium-labeled 1-hexylsilolane **17** (51.4 mg, 0.30 mmol, 1.5 equiv) and THF (0.2 mL). The vial was sealed and the mixture was stirred at 25 °C for 48 h. The vial was removed from the glove box, and the reaction mixture was passed through a short plug of silica gel, eluting with diethyl ether. The residue was purified by flash chromatography on silica gel (100% *n*-pentane) to give the desired product **19** (51.7 mg, 85%, C2:C3 > 20:1) as a colorless oil. R_f = 0.7 (100% *n*-pentane). ^1H NMR (700 MHz, C_6D_6): δ 7.68 – 7.65 (m, 2H), 7.41 (s, 1H), 7.18 (ddd, J = 8.0, 7.0, 1.0 Hz, 1H), 7.08 (ddd, J = 8.0, 7.0, 1.0 Hz, 1H), 1.78 – 1.70 (m, 2H), 1.68 – 1.60 (m, 2H), 1.47 – 1.41 (m, 2H), 1.36 – 1.31 (m, 2H), 1.31 – 1.21 (m, 4H), 1.03 – 0.96 (m, 2H), 0.94 – 0.90 (m, 2H), 0.89 (t, J = 7.3 Hz, 3H), 0.86 – 0.79 (m, 2H). The analytical data are in accordance with those reported.¹⁰

¹⁰ Fallon, T.; Oestreich, M. *Angew. Chem., Int. Ed.* **2015**, 54, 12488–12491

Synthesis of 3-(cyclopropylmethyl)-1-methyl-1H-indole (S2):



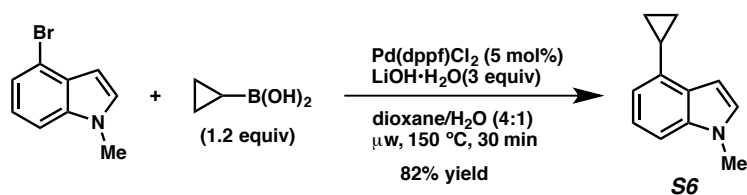
To a stirring solution of indole (1.17 g, 10 mmol) in CH_2Cl_2 (20 mL) was added SnCl_4 (1.44 mL, 12 mmol) in a single portion via syringe at 0 °C. The solution was allowed to warm to room temperature and stirred for 30 min, then cyclopropanecarbonyl chloride (10 mmol) was added in small portions to the suspension by syringe, followed by nitromethane (15 mL). The reaction mixture was stirred at 25 °C for 2 h, after which ice-water (30 mL) was slowly added. The mixture was then filtered, extracted with ethyl acetate (50 mL), dried over Na_2SO_4 , and concentrated at reduced pressure to give the product **S4** as a yellow solid, which was used directly for next step.¹¹

To a solution of crude **S4** in Et_2O (50 mL) was added LiAlH_4 (0.69 g, 20 mmol) in small portions, and the mixture refluxed overnight. The reaction was cooled to 0 °C, diluted with Et_2O (40 mL), and quenched with water (0.76 mL)/15% NaOH aqueous (0.76 mL)/water (2.28 mL). The mixture was stirred for 1 h, dried over Na_2SO_4 , concentrated at reduced pressure, and purified by silica gel flash chromatography (10% Et_2O in hexanes) to give 3-(cyclopropylmethyl)-1H-indole **S5** (0.63 g, 3.7 mmol) as a yellow oil.

To a dried flask with NaH (60% dispersion in oil, 178 mg, 4.4 mmol) and THF (15 mL) was added the THF (15 mL) solution of **S5** (630 mg, 3.7 mmol) dropwise by syringe at 0 °C. After the mixture was stirred at 0 °C for 30 min, MeI (0.35 mL, 5.6 mmol) was added slowly. This mixture was stirred overnight, quenched with aqueous NH_4Cl , extracted with Et_2O (30 mL x 3), and dried over Na_2SO_4 . The solvents were removed under

¹¹ Ottoni, O; Neder, A de V. F.; Dias, A. K. B; Cruz, R. P. A.; A.; Aquino, L. B. *Org. Lett.* **2001**, 3, 1005–1007.

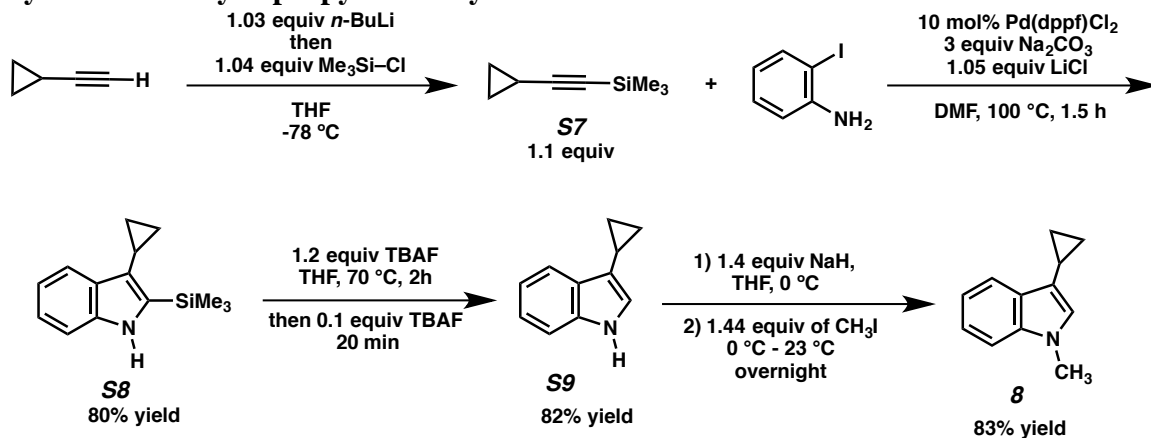
reduced pressure and the crude mixture was purified by silica gel flash chromatography (10% CH₂Cl₂ in hexanes) to give 3-(cyclopropylmethyl)-1-methyl-1*H*-indole **S2** (0.59 g, 32% yield over three steps) as a colorless oil. R_f = 0.4 (10% CH₂Cl₂ in hexanes); ¹H NMR (400 MHz, Chloroform-*d*) δ 7.70 (dt, J = 7.9, 1.1 Hz, 1H), 7.37 (dt, J = 8.3, 1.0 Hz, 1H), 7.31 (m, J = 6.9, 1.1 Hz, 1H), 7.19 (ddd, J = 8.0, 6.9, 1.2 Hz, 1H), 7.01 (s, 1H), 3.82 (s, 3H), 2.77 (d, J = 6.7 Hz, 2H), 1.18 (ttt, J = 8.0, 6.7, 4.9 Hz, 1H), 0.66 – 0.59 (m, 2H), 0.39 – 0.26 (m, 2H); ¹³C NMR (101 MHz, Chloroform-*d*) δ 137.12, 128.13, 126.26, 121.52, 119.24, 118.66, 115.12, 109.20, 32.67, 30.03, 11.50, 5.03. IR (Neat Film NaCl) 3073, 3054, 2999, 2905, 2837, 1615, 1552, 1483, 1472, 1423, 1371, 1355, 1327, 1293, 1253, 1235, 1201, 1156, 1129, 1057, 1013, 975, 929, 884, 828, 803, 737 cm⁻¹; HRMS (MM: ESI-APCI+) calc'd for C₁₃H₁₅N [M+H]⁺: 186.1277, found: 186.1277.



To a 20 mL microwave vial was added Pd(dppf)Cl₂ (367 mg, 0.5 mmol, 5 mol%), lithium hydroxide mono-hydrate (1.26 g, 30 mmol, 3 equiv), 4-bromo-1-methyl-1*H*-indole (2.10g, 10 mmol), and cyclopropylboronic acid (1.03 g, 12 mmol, 1.2 equiv), followed by dioxane (10 mL) and degassed H₂O (2.5 mL). The vial is purged with N₂ for 15 min, then heated to 150 °C for 30 minutes in a Biotage Initiator 2.5 microwave reactor under normal absorption mode. The vial was cooled and the solution concentrated under reduced pressure, diluted with ethyl acetate (100 mL), washed with saturated sodium bicarbonate (50 mL) then brine (50 mL), dried over Na₂SO₄, and concentrated under reduced pressure. The crude mixture was purified by silica gel flash chromatography (2→10% CH₂Cl₂ in hexanes) to give 4-cyclopropyl-1-methyl-1*H*-indole **S6** (1.39 g, 81% yield) as a white solid. R_f = 0.2 (10% CH₂Cl₂ in hexanes); ¹H NMR (400 MHz, Chloroform-*d*) δ 7.20 – 7.13 (m, 2H), 7.07 (d, J = 3.1 Hz, 1H), 6.79 – 6.70 (m, 1H), 6.67 (d, J = 3.1 Hz, 1H), 3.80 (s, 3H), 2.26 (ttt, J = 8.5, 5.2, 0.7 Hz, 1H), 1.08 – 0.95 (m, 1H), 0.92 – 0.80 (m, 1H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 136.52, 136.17, 128.53, 128.33, 121.84, 114.59, 106.83, 99.40, 33.09, 13.20, 7.76. IR (Neat Film NaCl) 3002, 2943, 1581, 1498, 1458, 1418, 1336, 1291, 1252, 1154, 1088, 1034, 961, 811, 786, 746,

715 cm^{-1} ; HRMS (MM: ESI-APCI+) calc'd for $\text{C}_{12}\text{H}_{13}\text{N}$ $[\text{M}+\text{H}]^+$: 172.1121, found: 172.1120.

Synthesis of 3-cyclopropyl-1-methyl-1*H*-indole **8**



(cyclopropylethynyl)trimethylsilane S7: Synthesis was conducted by a slight modification of the reported procedure.¹² To a stirring solution of cyclopropylacetylene (1.44 g, 21.8 mmol, 1 equiv) in dry THF (7 mL) at -78°C was added *n*-BuLi (8.95 mL of 2.5 M in THF, 22.4 mmol, 1.03 equiv) dropwise via syringe. The solution was allowed to stir for 30 minutes at -78°C , after which TMS-Cl (freshly distilled from CaH_2 , 2.90 mL, 22.8 mmol, 1.04 equiv) was added dropwise and the solution was stirred at -78°C for 1 hour. The reaction was then allowed to warm to room temperature, diluted with diethyl ether, and filtered through a pad of Na_2SO_4 layered on silica gel, eluting 1:4 Et_2O : pentane. The filtrate was concentrated in vacuo and then carried on crude.

¹² Kozhushkov, S. I.; Wagner-Gillen, K.; Khlebnikov, A. F.; de Meijere, A. *Synthesis* **2010**, 2010, 3967–3973.

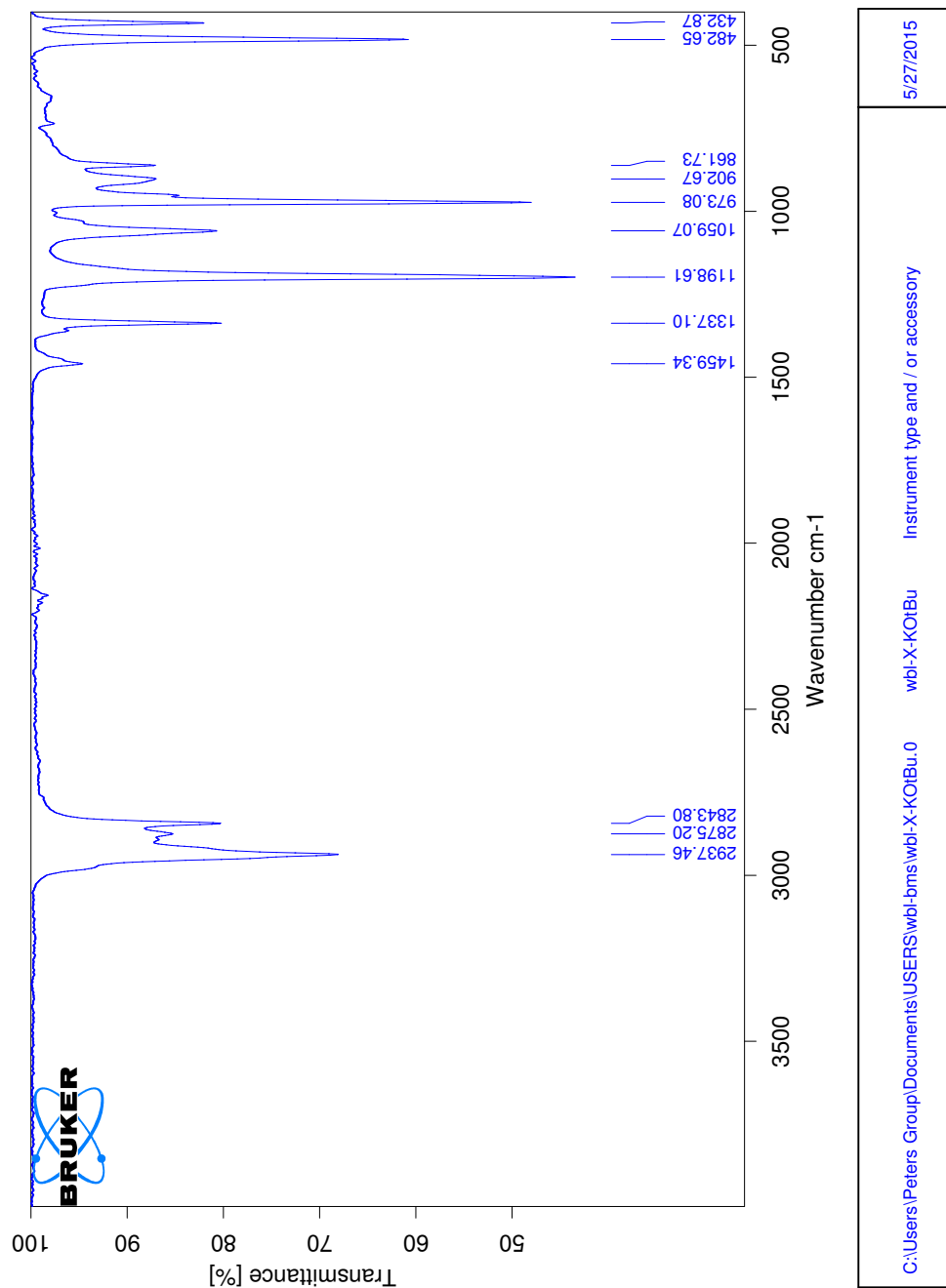
3-cyclopropyl-2-(trimethylsilyl)-1*H*-indole S8 and 3-cyclopropyl-1*H*-indole S9 were synthesized following known procedure using **S7** and 2-iodoaniline.¹³

3-cyclopropyl-1-methyl-1*H*-indole 8: To a round-bottom flask equipped with a magnetic stirring bar was added NaH (60 % dispersion in mineral oil, 155 mg, 3.9 mmol, 1.4 equiv) and **S9** (440 mg, 2.8 mmol, 1 equiv). The flask was placed in an ice bath and THF was added while stirring. The reaction was stirred at 0 °C for 45 minutes and then at 23 °C for 15 minutes. The reaction was again placed in an ice bath and Me-I (250 µL, 4 mmol, 1.4 equiv) was added dropwise. This mixture was stirred overnight, quenched with aqueous NH₄Cl, extracted with Et₂O (30 mL x 3), and dried over Na₂SO₄. The solvents were removed under reduced pressure and the crude mixture was purified by silica gel flash chromatography (5→10% CH₂Cl₂ in hexanes) to give 3-cyclopropyl-1-methyl-1*H*-indole **8** (398 mg, 83% yield) *R*_f = 0.35 (10% CH₂Cl₂ in hexanes) ¹H NMR (400 MHz, Chloroform-*d*) δ 7.74 (dt, *J* = 7.9, 0.9 Hz, 1H), 7.31 – 7.27 (m, 1H), 7.25 – 7.20 (m, 1H), 7.12 (t, *J* = 8.0 Hz, 1H), 6.76 (s, 1H), 3.72 (s, 3H), 2.11 – 1.87 (m, 1H), 0.92 – 0.85 (m, 2H), 0.71 – 0.56 (m, 2H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 137.14, 128.59, 125.43, 121.73, 119.36, 118.74, 117.74, 109.25, 32.69, 6.19.; HRMS (MM: ESI-APCI+) calc'd for C₁₂H₁₃N [M+H]⁺: 172.1121, found: 172.1119.

¹³ (a) Zemolka, S.; Schunk, S.; Englberger, W.; Kogel, B.-Y.; Linz, K.; Schick, H.; Sonnenschein, H.; Graubaum, H.; Hinze, C. (Gruenthal GmbH, Aachen, Germany) Substituted heteroaryl derivatives. U.S. Patent 8,138,187, March 20, 2012. (b) Penoni, A.; Palmisano, G.; Zhao, Y.-L.; Houk, K. N.; Volkman, J.; Nicholas, K. M. *J. Am. Chem. Soc.* **2008**, *131*, 653–661

FTIR Spectra:

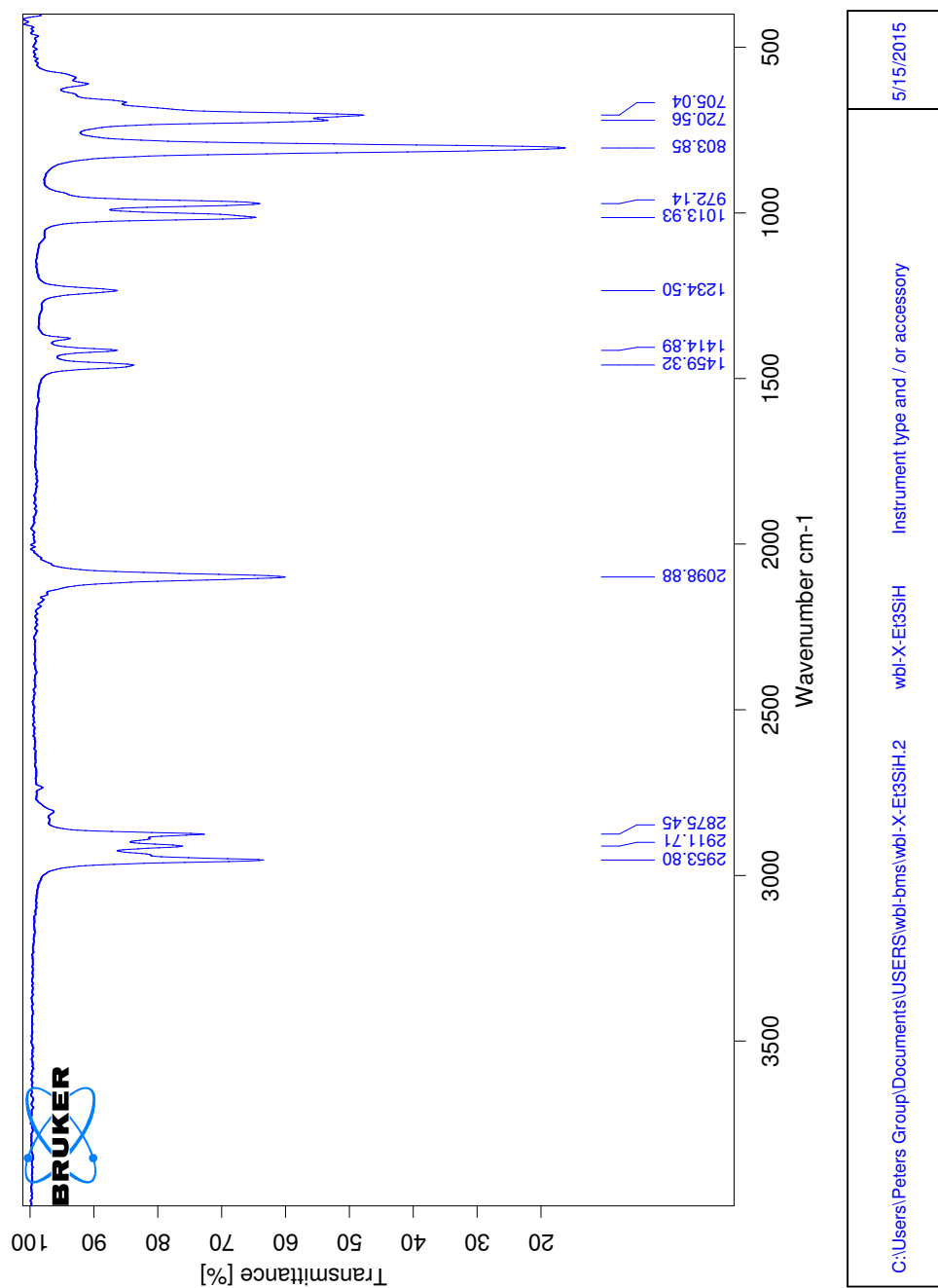
Pure KOt-Bu:

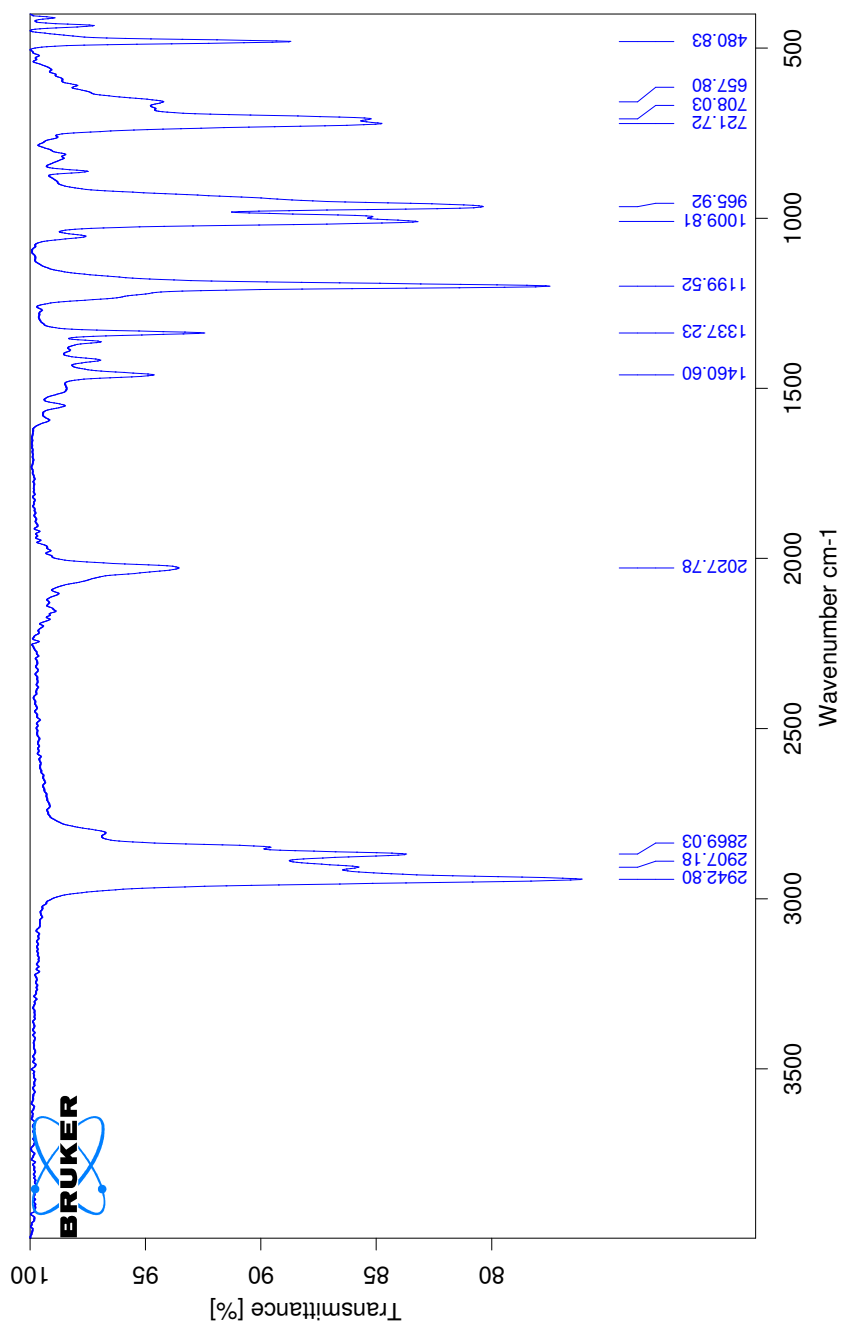
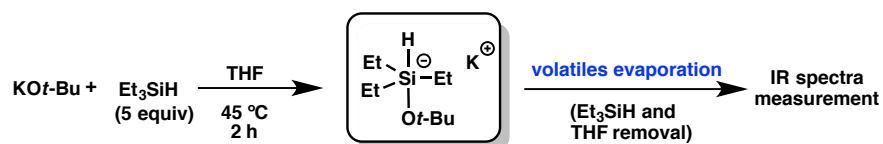


C:\Users\Peters Group\Documents\USERS\wbi-bms\wbi-X-KOtBu.0 wbi-X-KOtBu Instrument type and / or accessory

5/27/2015

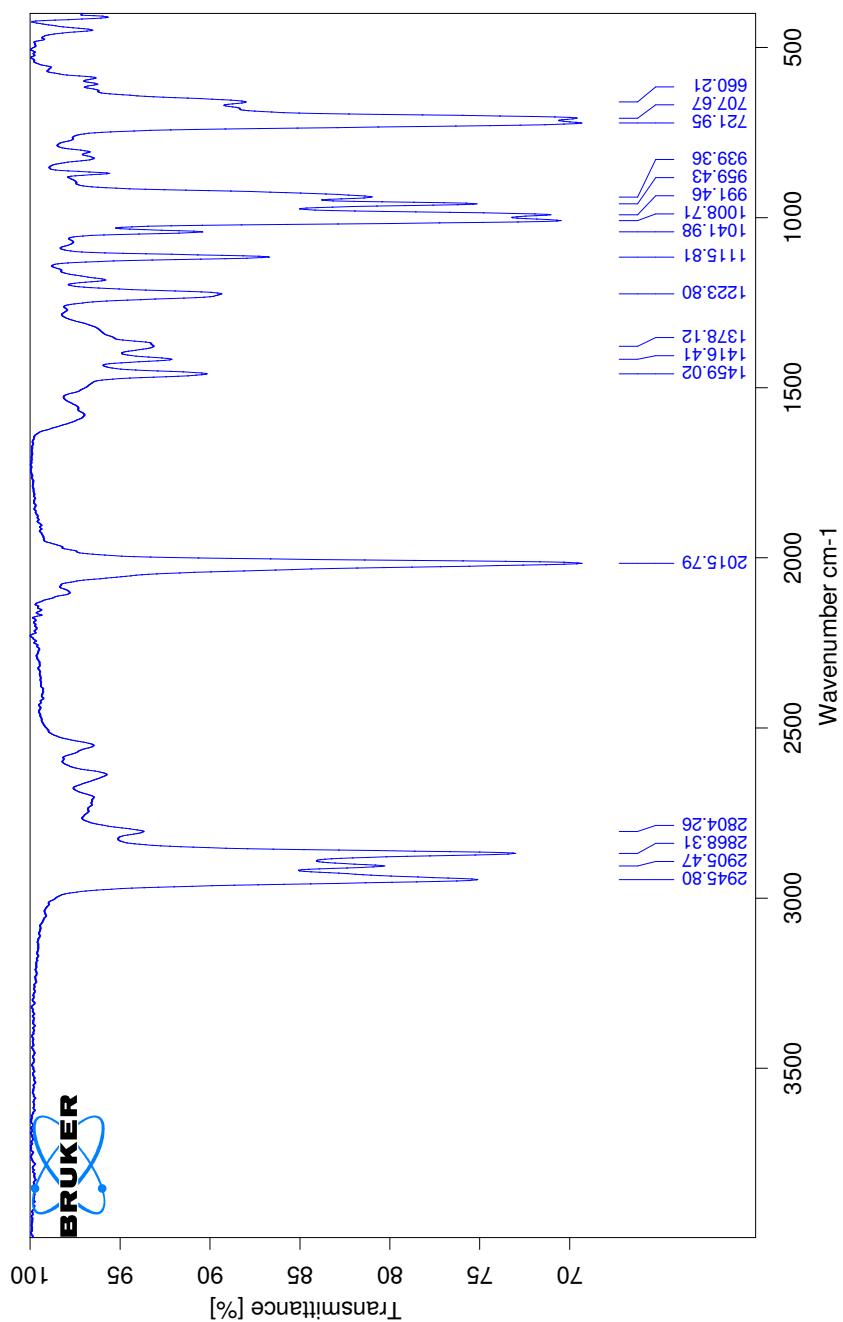
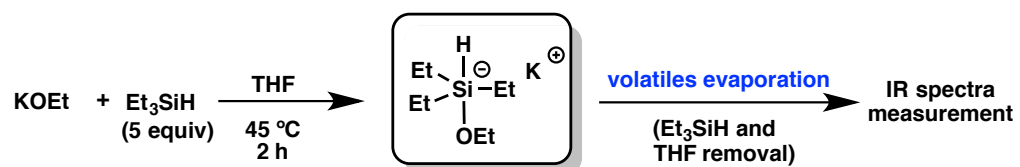
Pure Et₃SiH:





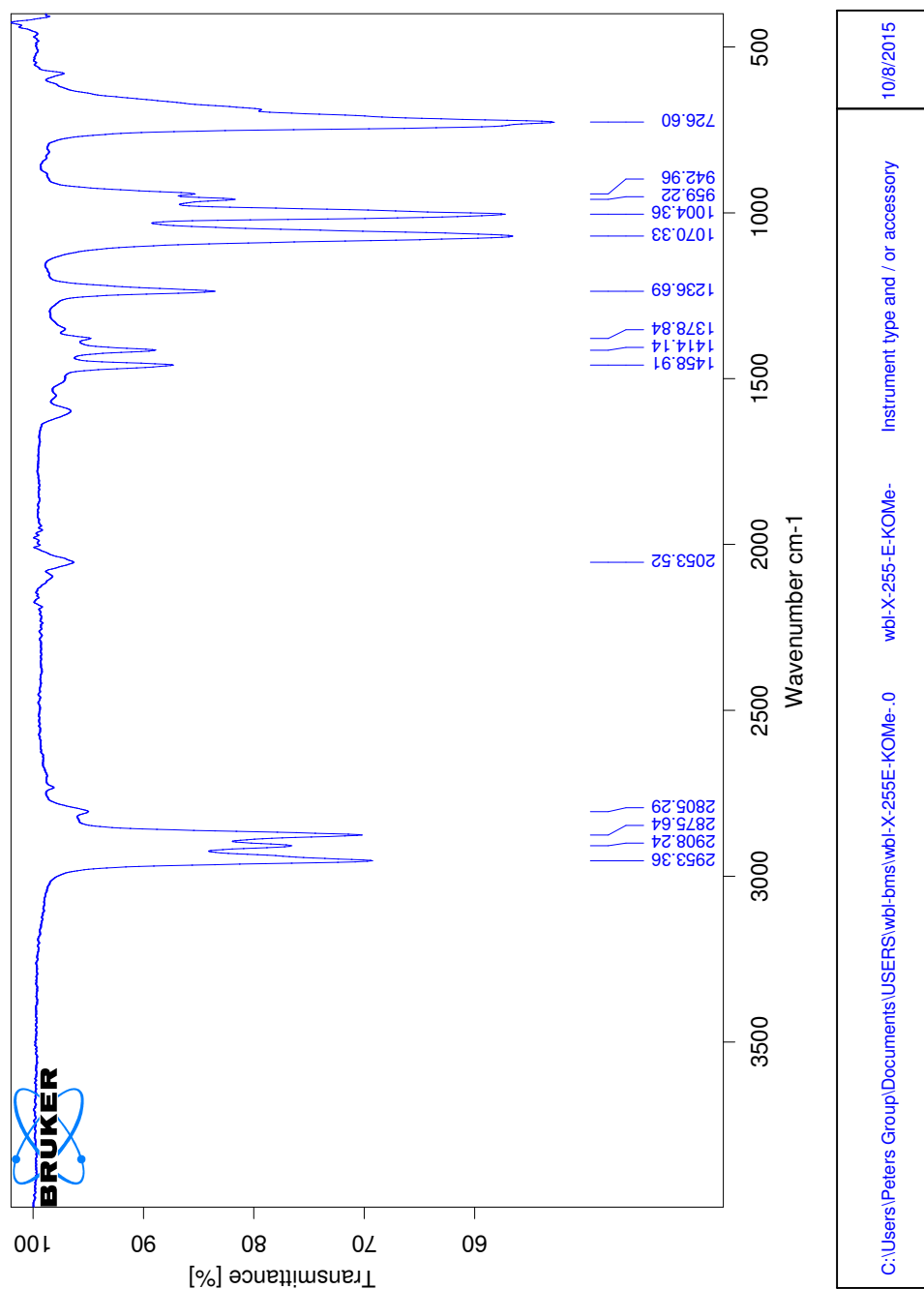
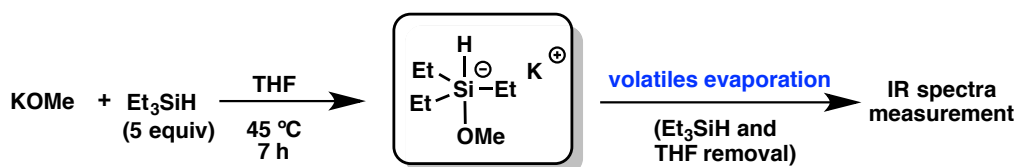
C:\Users\Peters Group\Documents\USERS\wbl-bms\wbl-X-255A.0 wbl-X-255-A Instrument type and / or accessory

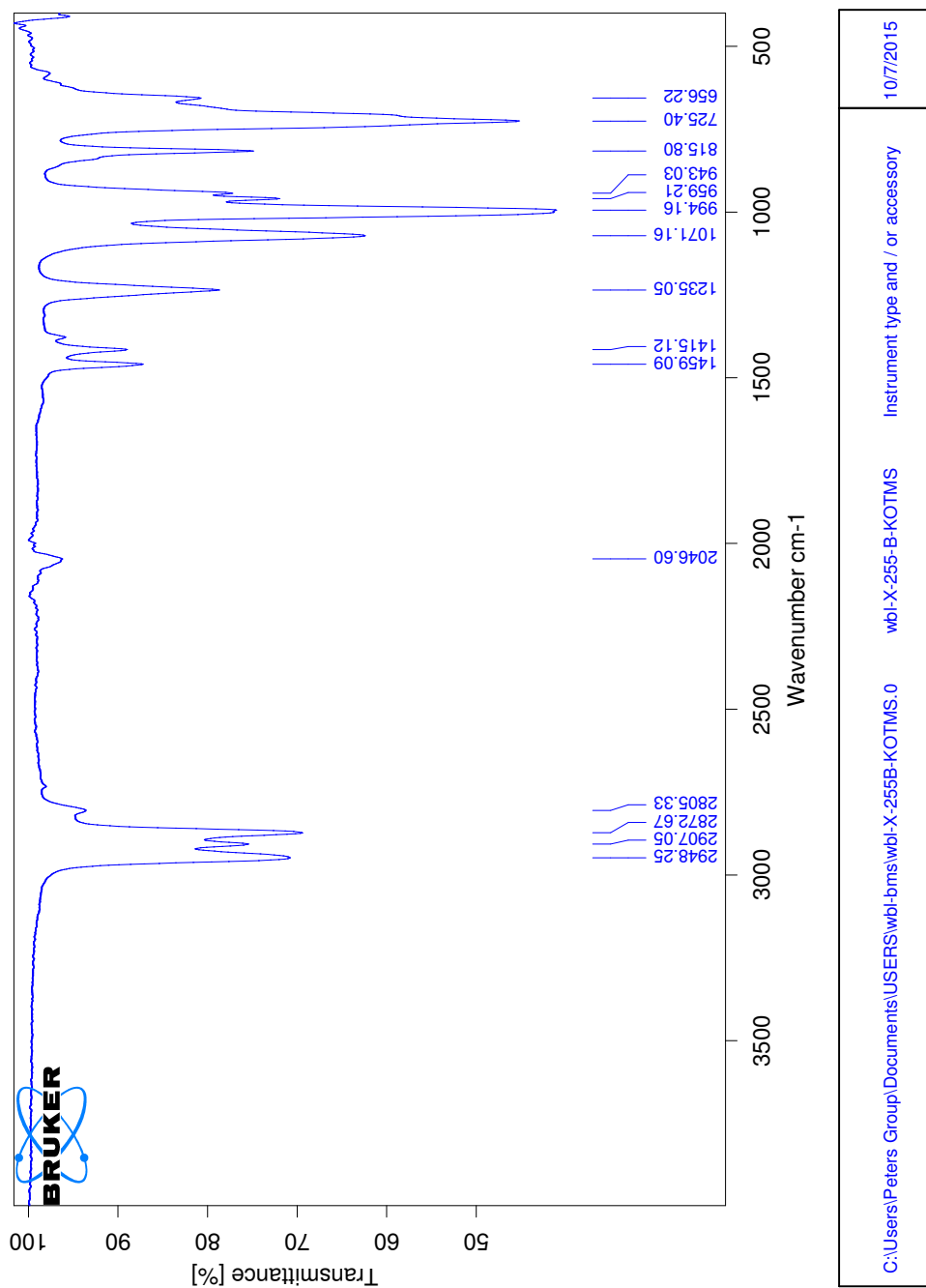
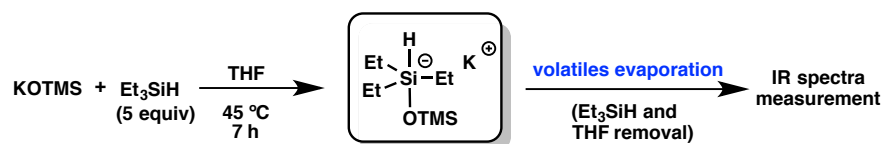
10/7/2015

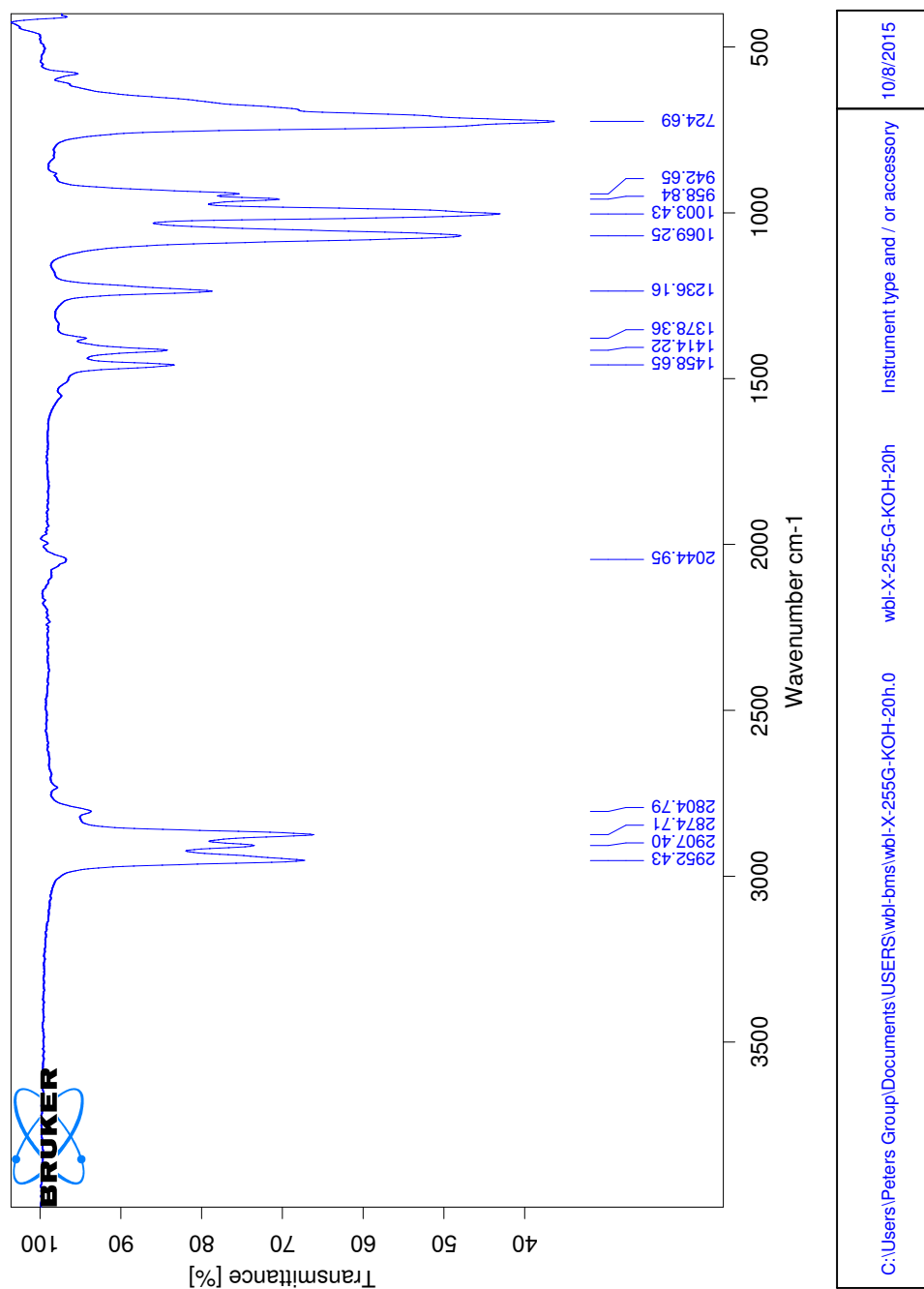
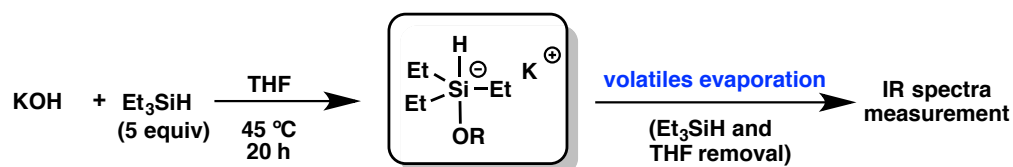


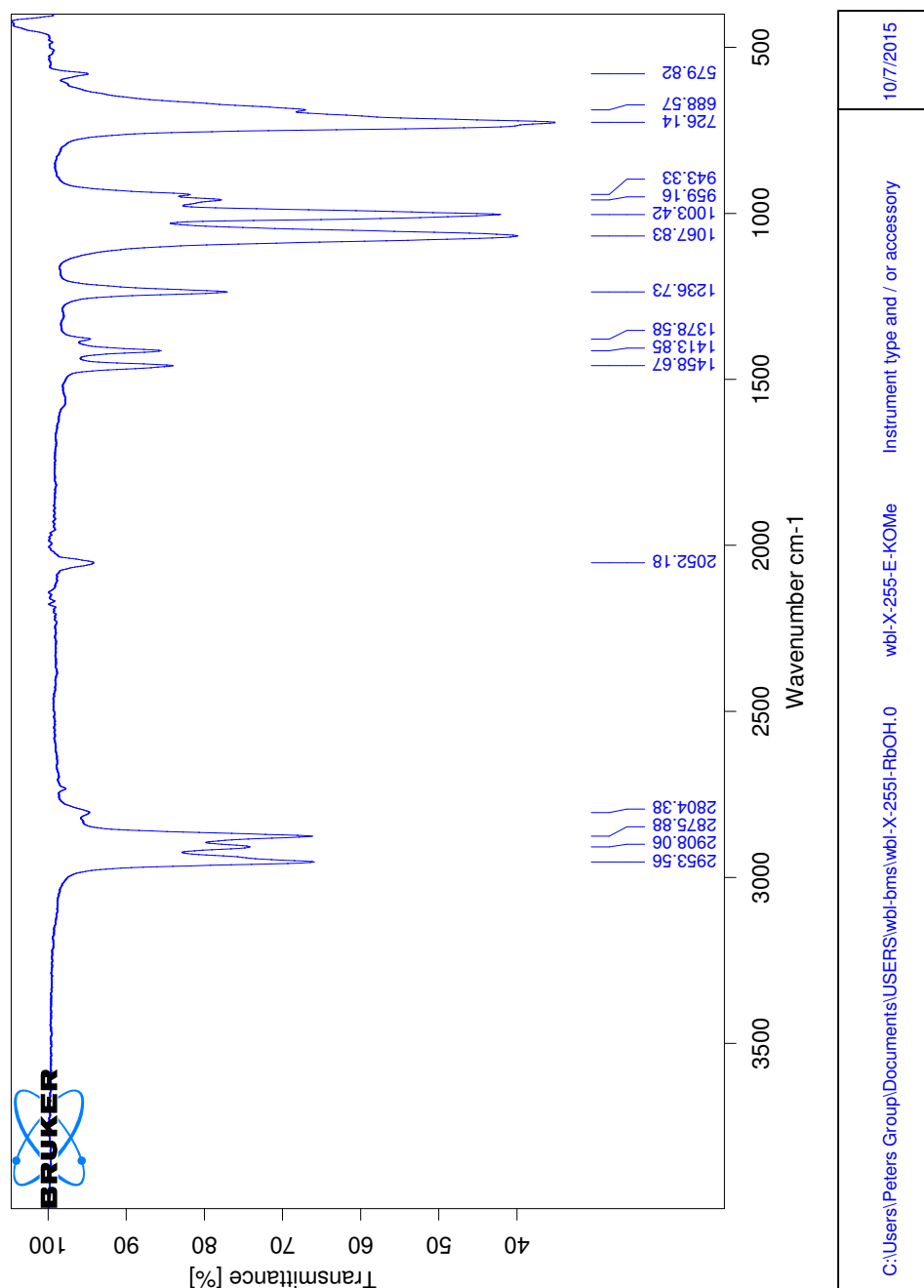
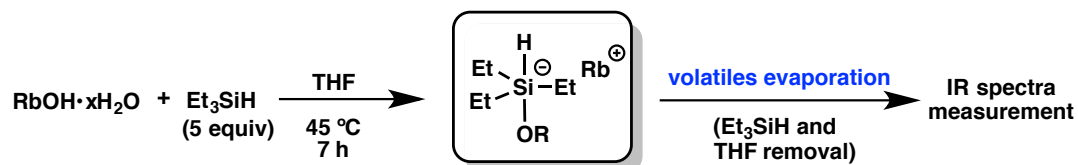
C:\Users\Peters Group\Documents\USERS\wbl-bms\wbl-X-255D-KOEt-.0 wbl-X-255-D-KOEt- Instrument type and / or accessory

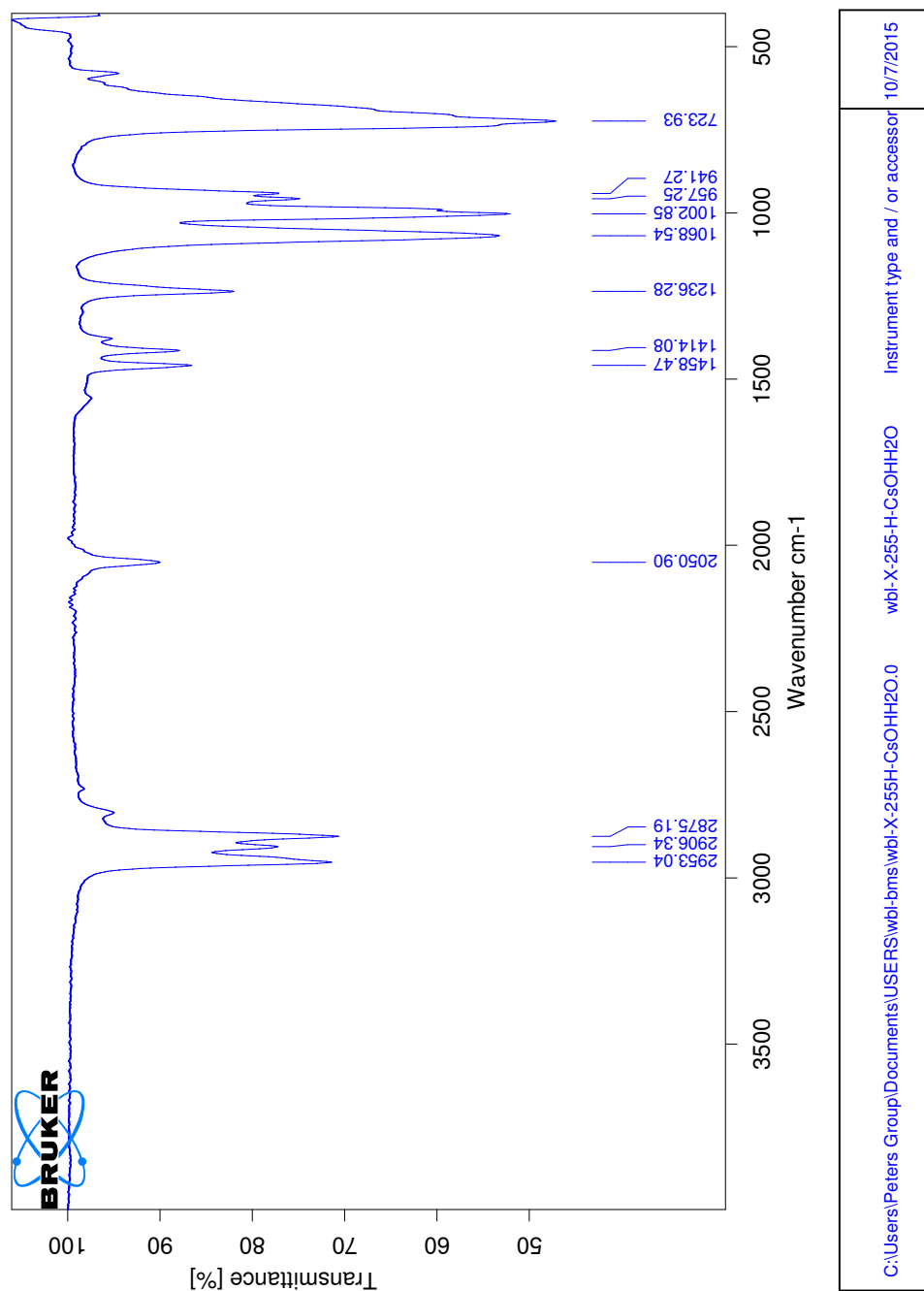
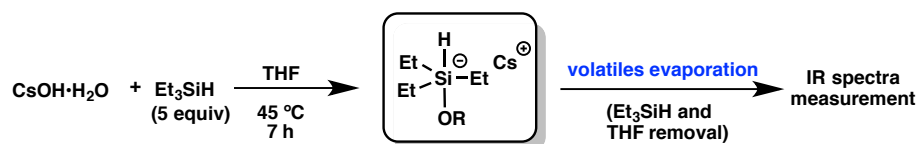
10/7/2015

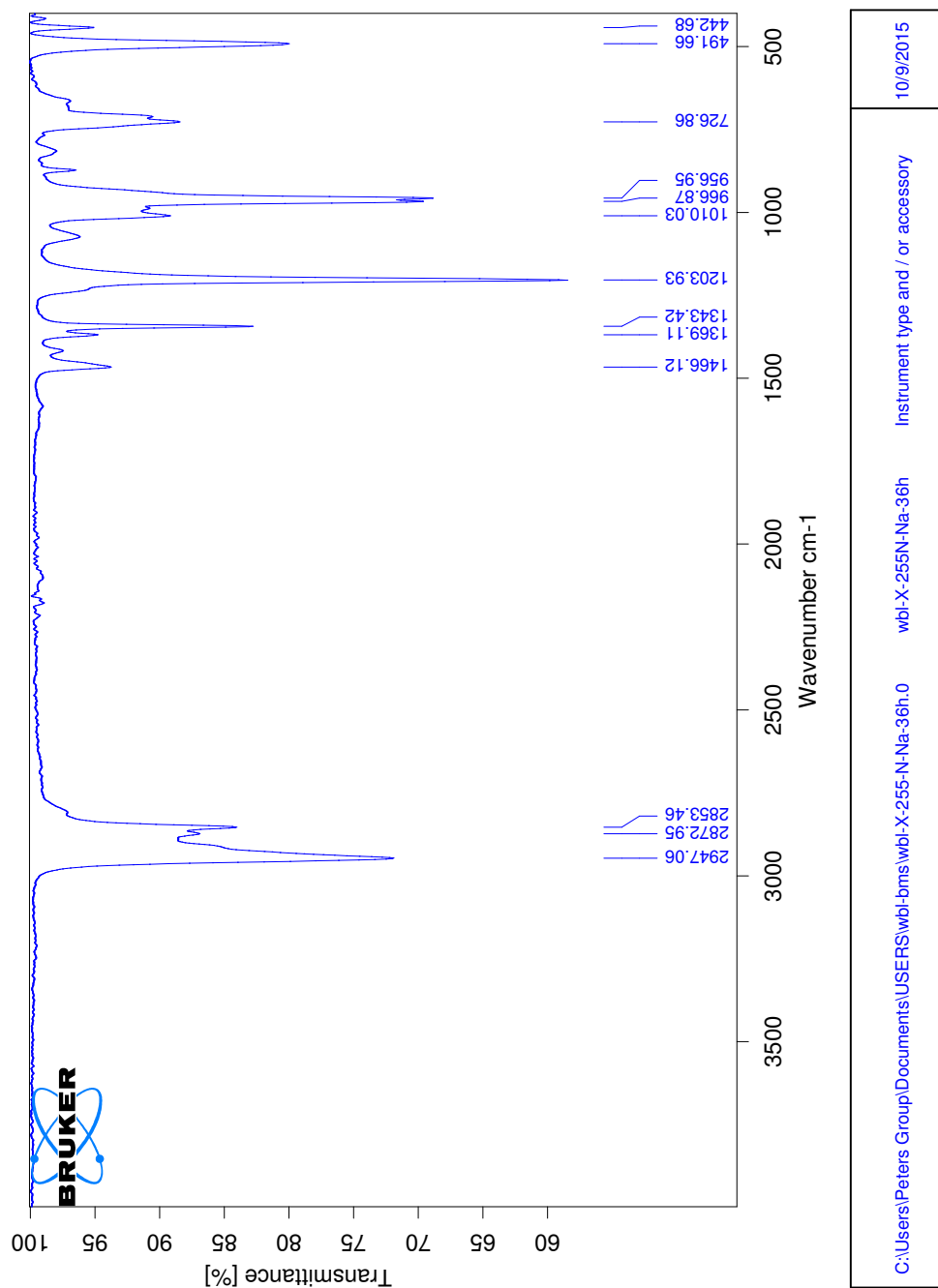
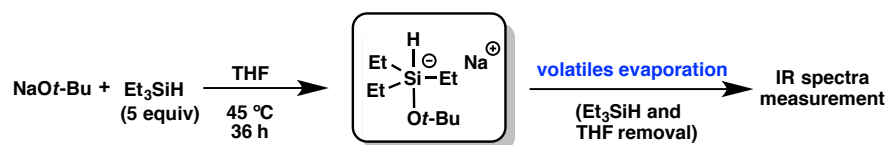


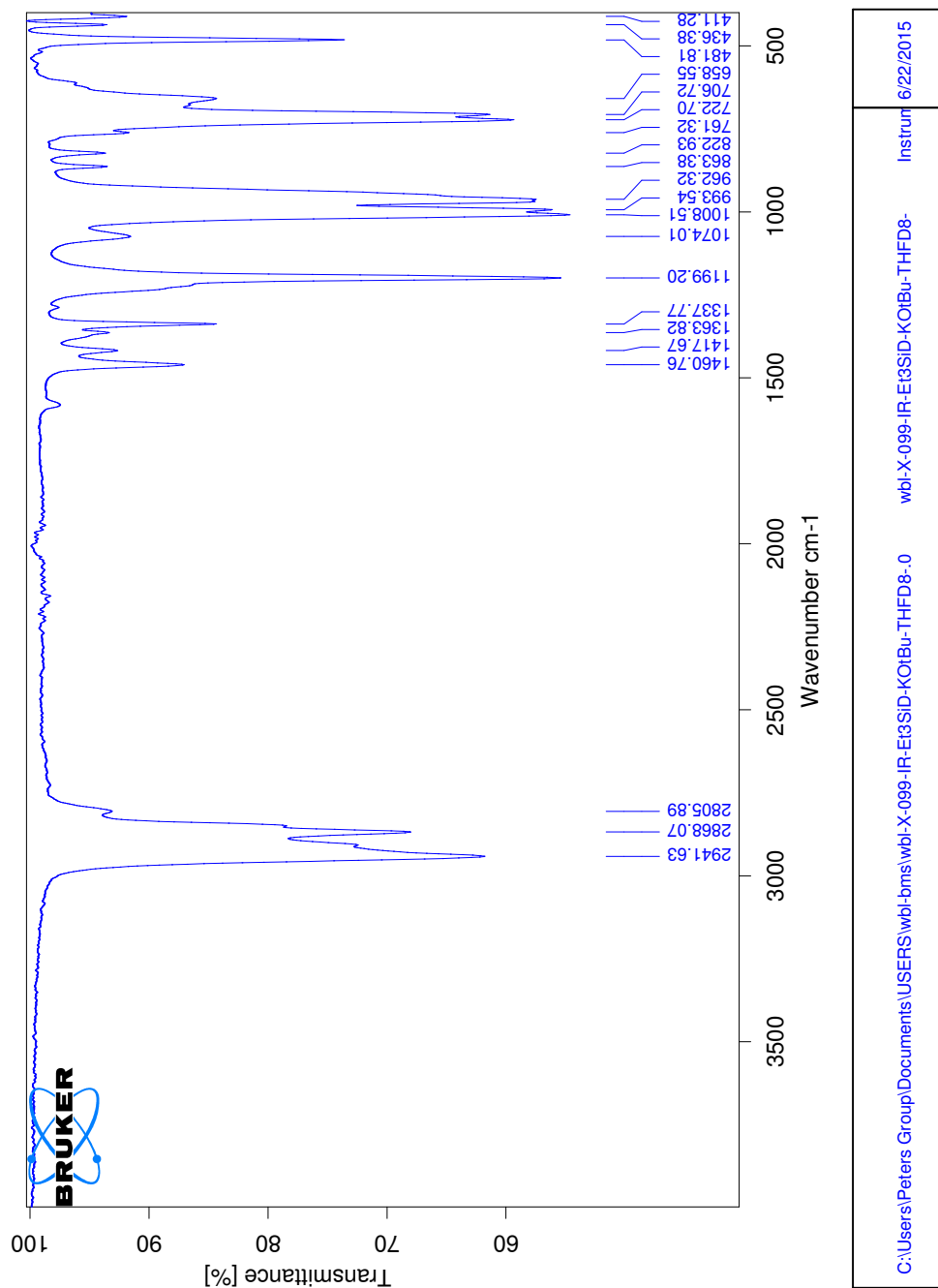
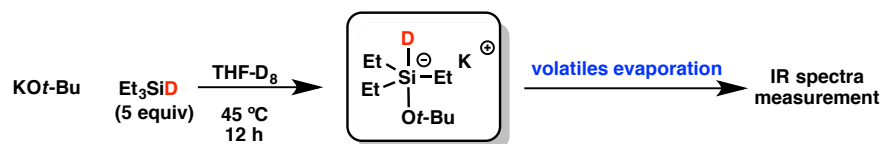


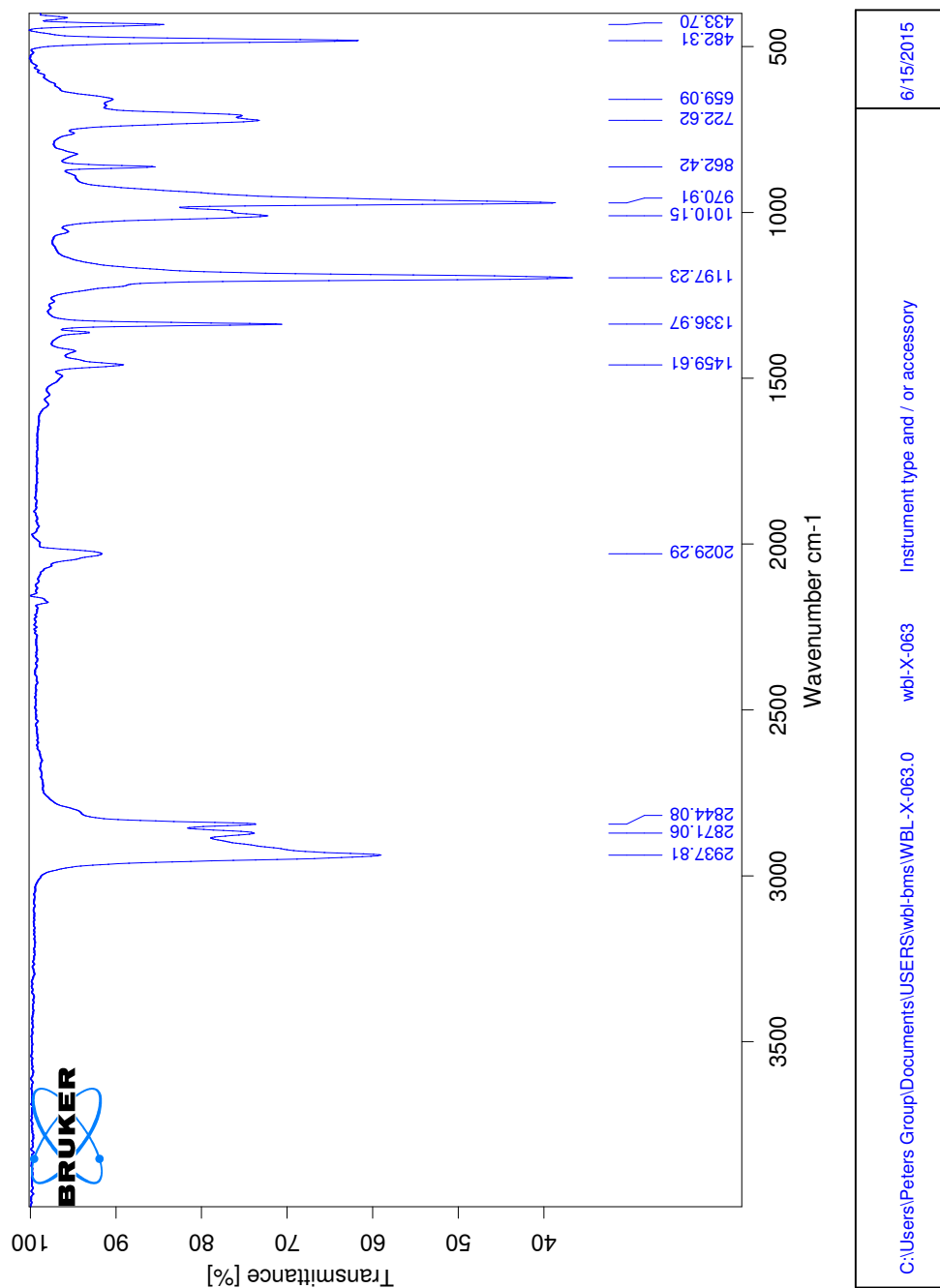
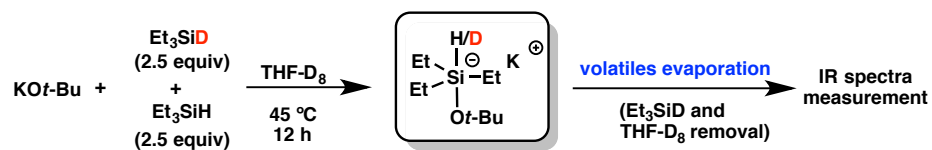


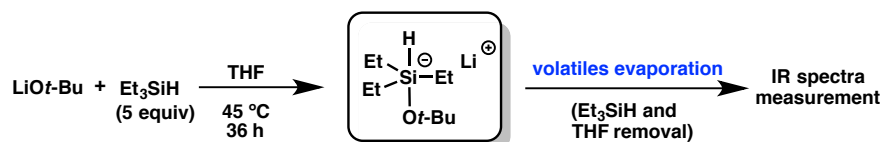




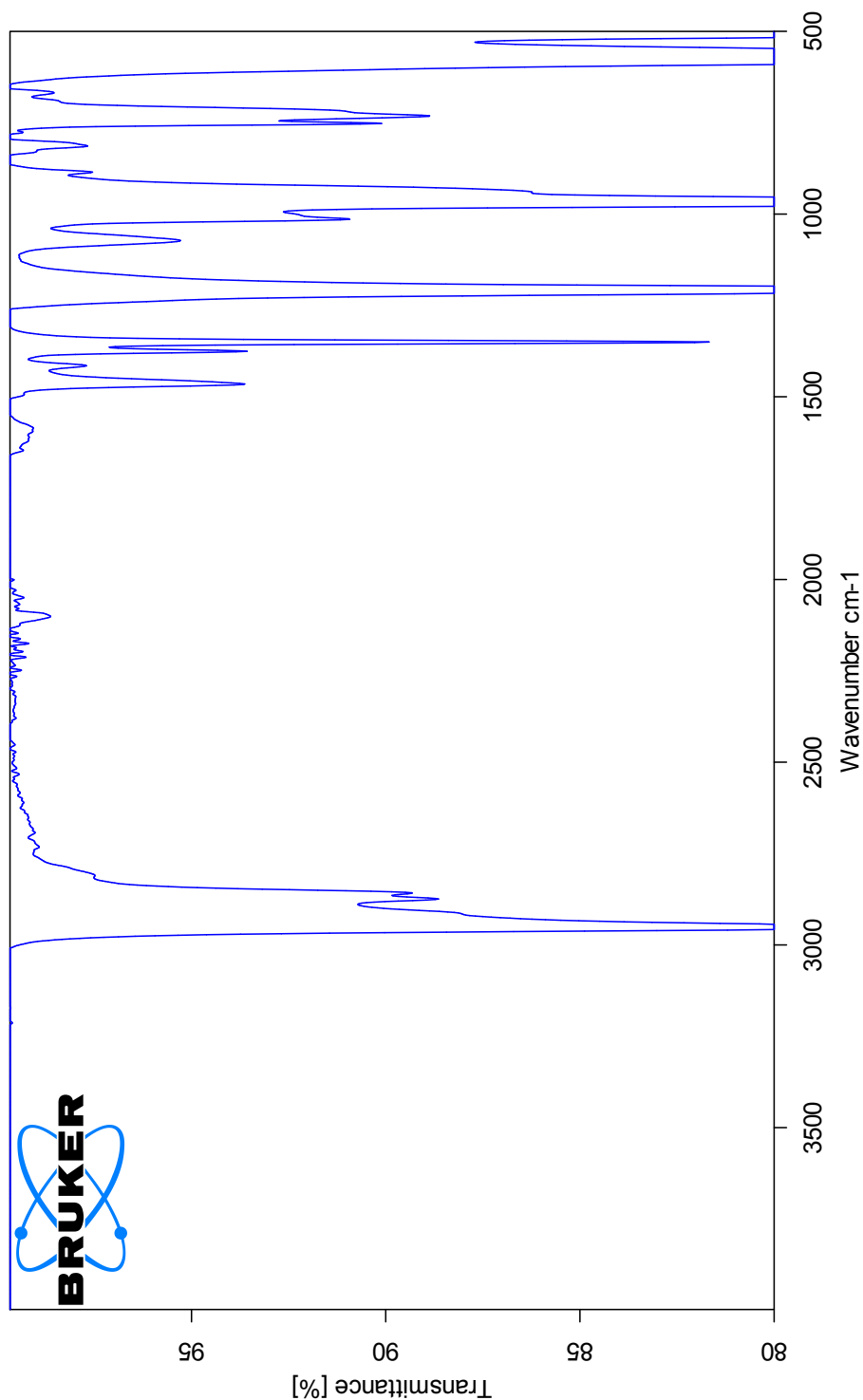








Note- small peak at 2101 cm^{-1} due to residual Et_3SiH

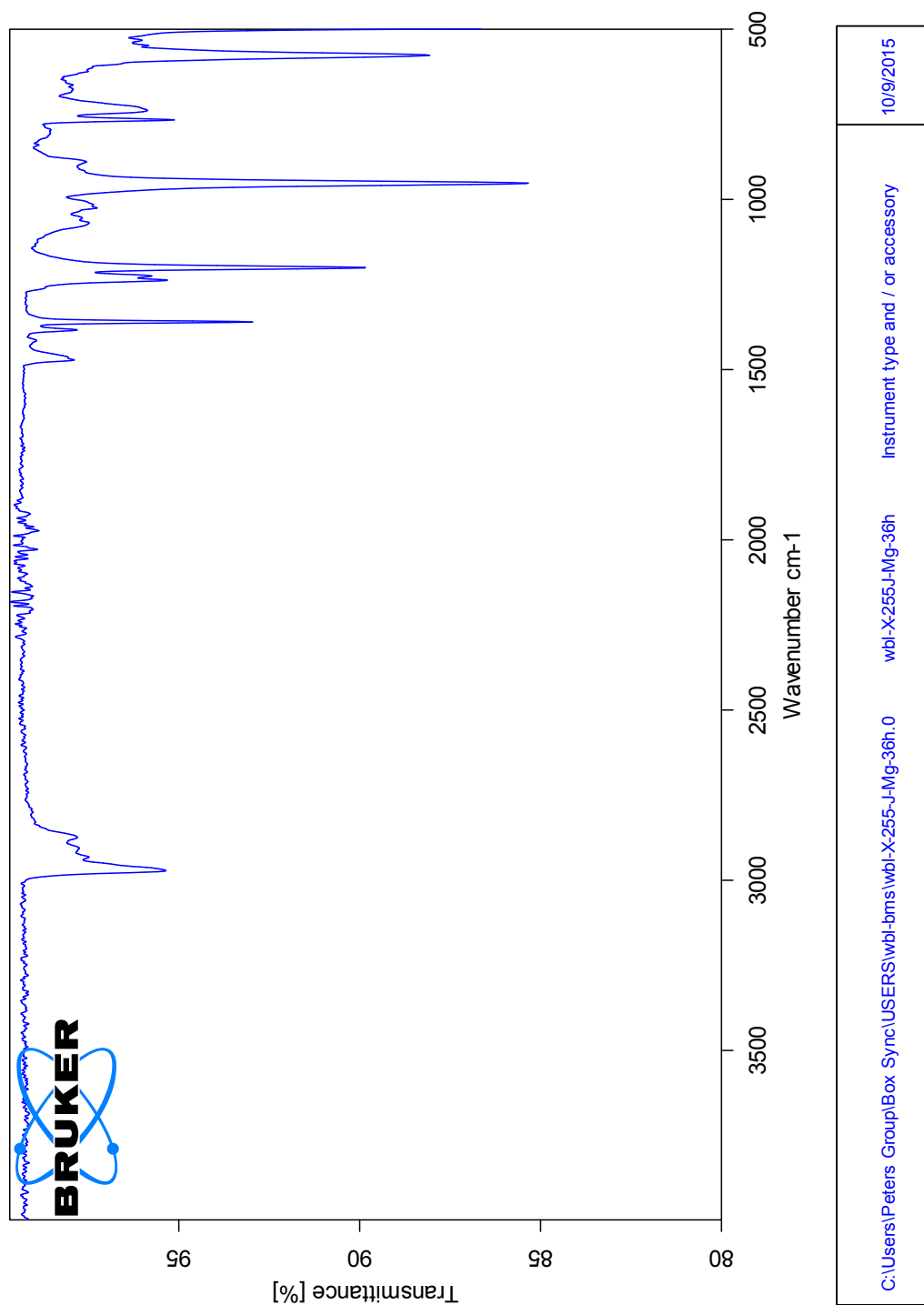
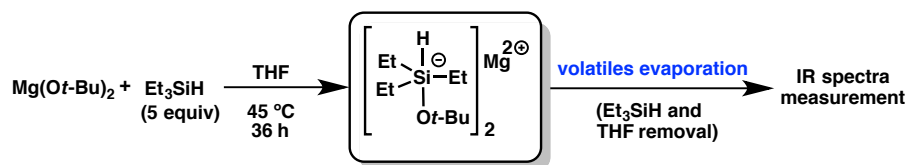


10/9/2015

Instrument type and / or accessory

wbi-X-255M-LI-36h-

C:\Users\Peters Group\Box Sync\USERS\wbi-bms\wbi-X-255-M-LI-36h-.1

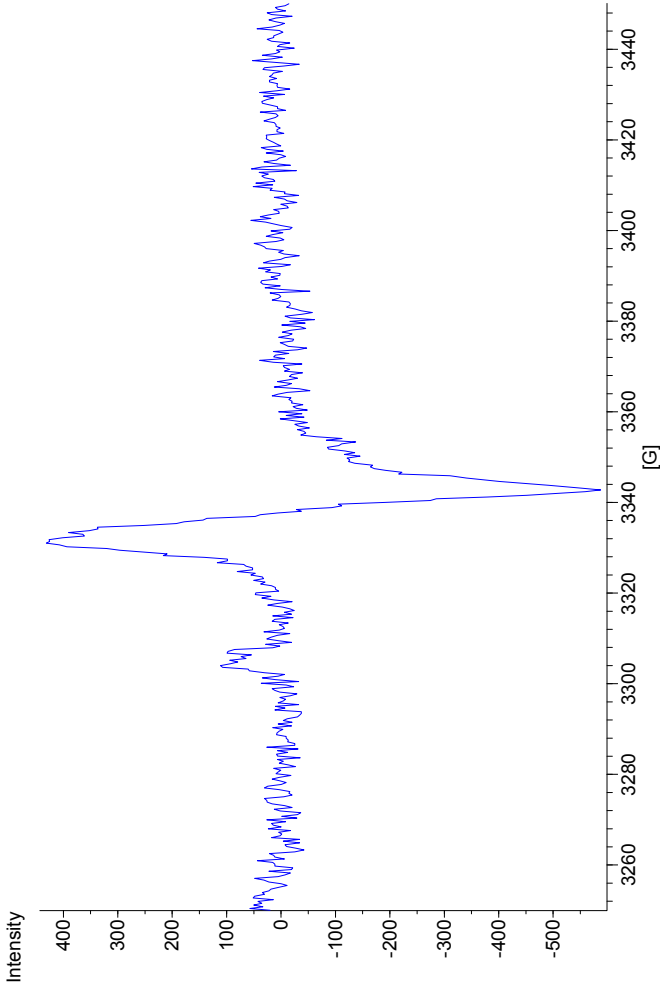


EPR Spectrum

WinEPR Acquisition

FileName: C:\Documents and Settings\EPR\Desktop\EPR Data All Users\Stoltz\wbl-IX-287-A-77k.par

Date: 06/20/2015 Time: 16:11



Parameter List

Operator: Bruker BioSpin GmbH
Resonator: c:\...\hs 4119 sept 2014.cal
Acq. Date: 05/04/2015
of Scans: 4

Field
Center Field: 3350.000 G
Sweep Width: 200.000 G
Resolution: 512 points

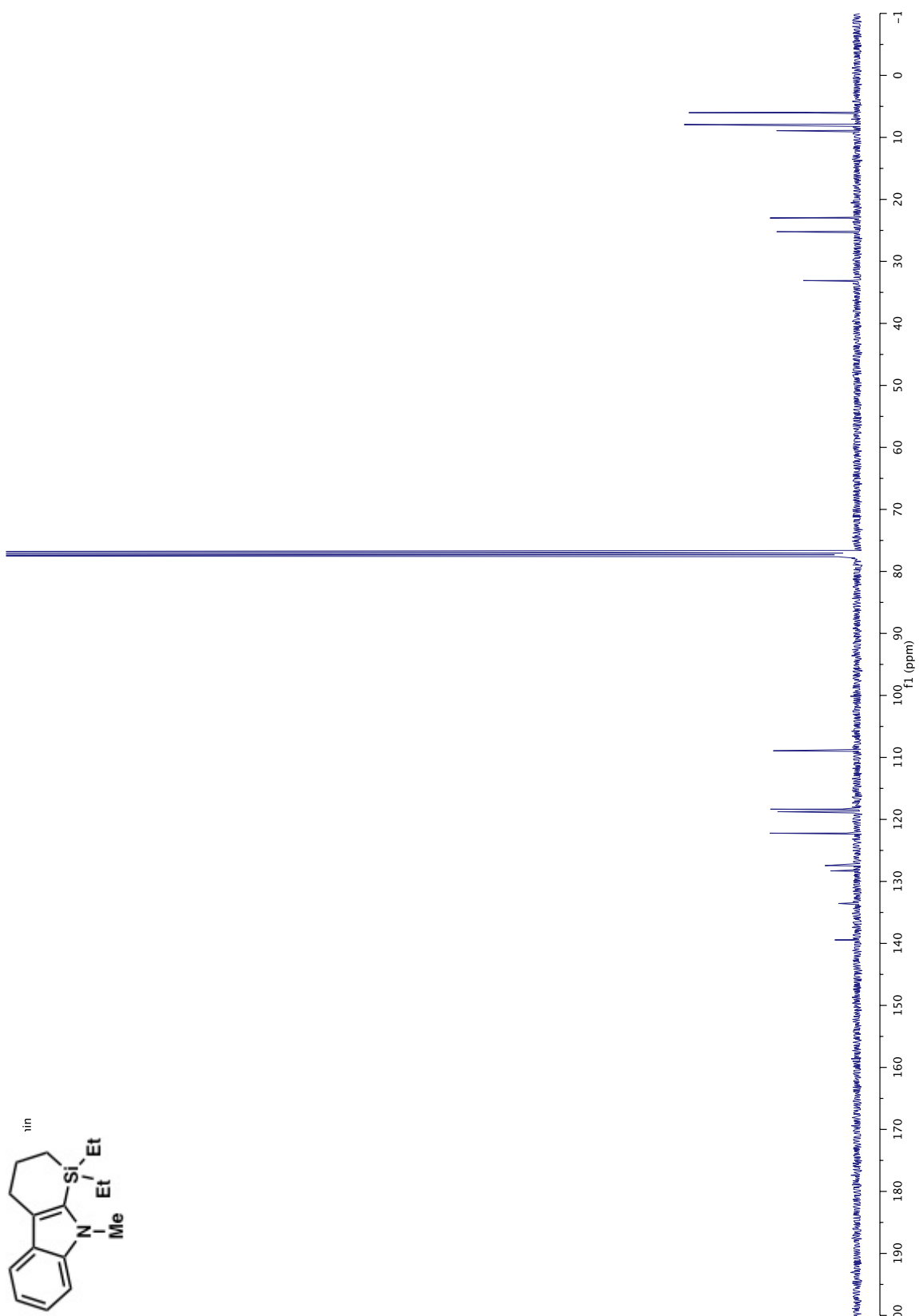
Microwave
Frequency: 9.377 GHz
Power: 2.036 mW

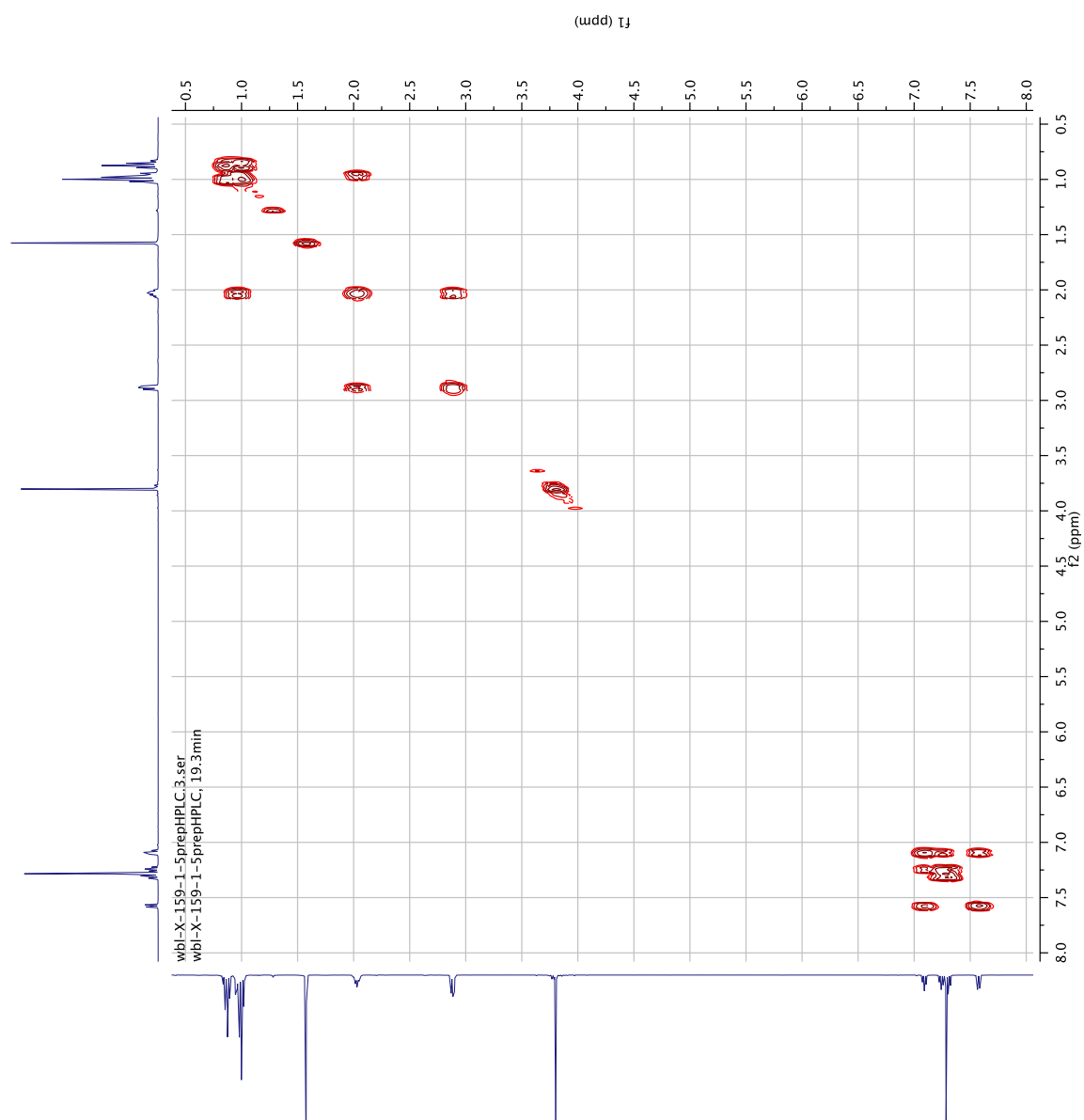
Receiver
Receiver Gain: 6.32e+003
Phase: 0.00 deg
Harmonic: 1
Mod. Frequency: 100.00 kHz
Mod. Amplitude: 2.00 G

Signal Channel
Conversion: 81.920 ms
Time Constant: 20.480 ms
Sweep Time: 41.943 s

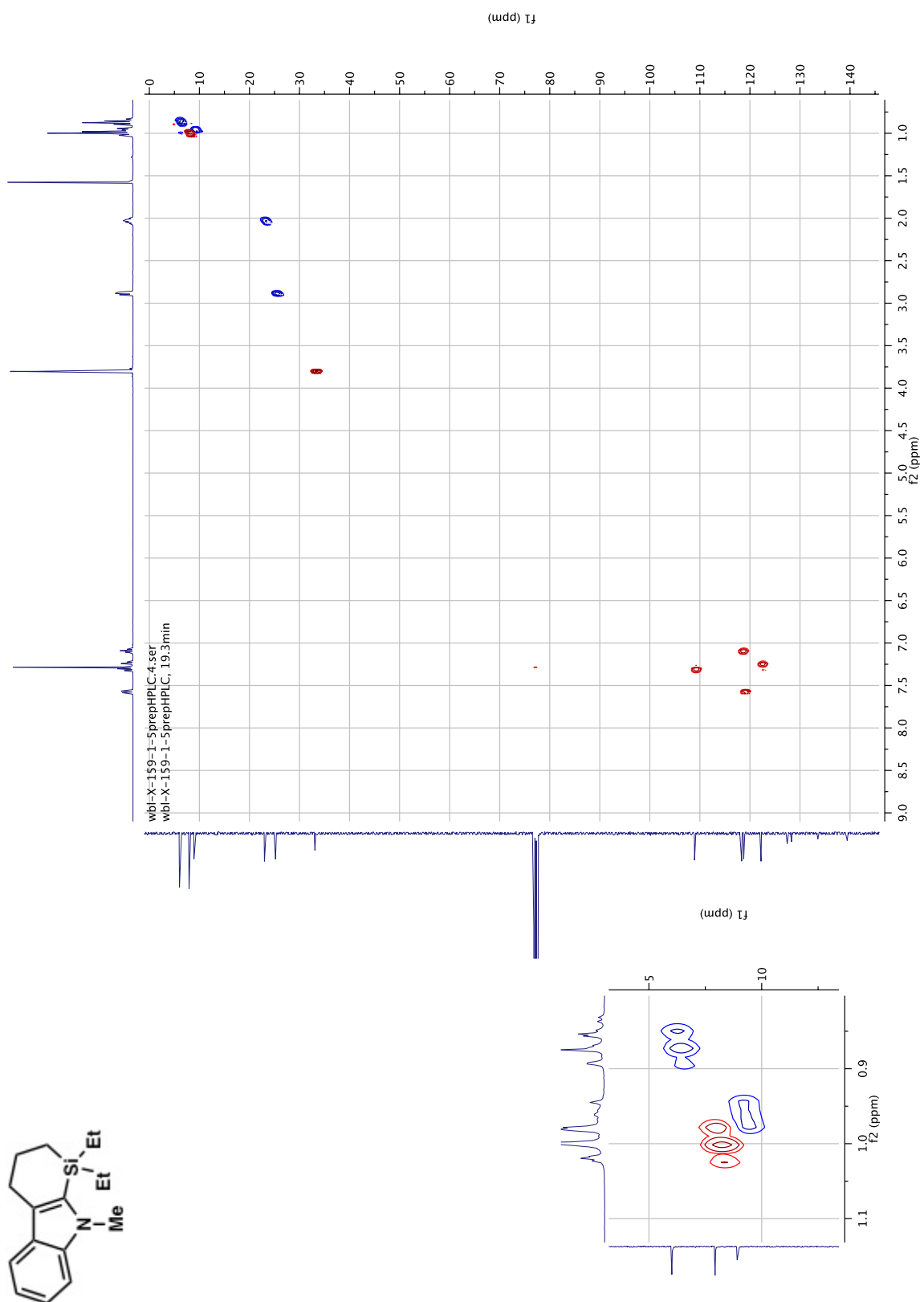
EPR Spectra of Et₃SiH and KOt-Bu

CC1(C)N(C2=CC=CC=C2C3=CC=CC=C3C4=CC=CC=C4C5=CC=CC=C5C6=CC=CC=C6C7=CC=CC=C7C8=CC=CC=C8C9=CC=CC=C9C10=CC=CC=C10C11=CC=CC=C11C12=CC=CC=C12C13=CC=CC=C13C14=CC=CC=C14C15=CC=CC=C15C16=CC=CC=C16C17=CC=CC=C17C18=CC=CC=C18C19=CC=CC=C19C20=CC=CC=C20C21=CC=CC=C21C22=CC=CC=C22C23=CC=CC=C23C24=CC=CC=C24C25=CC=CC=C25C26=CC=CC=C26C27=CC=CC=C27C28=CC=CC=C28C29=CC=CC=C29C30=CC=CC=C30C31=CC=CC=C31C32=CC=CC=C32C33=CC=CC=C33C34=CC=CC=C34C35=CC=CC=C35C36=CC=CC=C36C37=CC=CC=C37C38=CC=CC=C38C39=CC=CC=C39C40=CC=CC=C40C41=CC=CC=C41C42=CC=CC=C42C43=CC=CC=C43C44=CC=CC=C44C45=CC=CC=C45C46=CC=CC=C46C47=CC=CC=C47C48=CC=CC=C48C49=CC=CC=C49C50=CC=CC=C50C51=CC=CC=C51C52=CC=CC=C52C53=CC=CC=C53C54=CC=CC=C54C55=CC=CC=C55C56=CC=CC=C56C57=CC=CC=C57C58=CC=CC=C58C59=CC=CC=C59C60=CC=CC=C60C61=CC=CC=C61C62=CC=CC=C62C63=CC=CC=C63C64=CC=CC=C64C65=CC=CC=C65C66=CC=CC=C66C67=CC=CC=C67C68=CC=CC=C68C69=CC=CC=C69C70=CC=CC=C70C71=CC=CC=C71C72=CC=CC=C72C73=CC=CC=C73C74=CC=CC=C74C75=CC=CC=C75C76=CC=CC=C76C77=CC=CC=C77C78=CC=CC=C78C79=CC=CC=C79C80=CC=CC=C80C81=CC=CC=C81C82=CC=CC=C82C83=CC=CC=C83C84=CC=CC=C84C85=CC=CC=C85C86=CC=CC=C86C87=CC=CC=C87C88=CC=CC=C88C89=CC=CC=C89C90=CC=CC=C90C91=CC=CC=C91C92=CC=CC=C92C93=CC=CC=C93C94=CC=CC=C94C95=CC=CC=C95C96=CC=CC=C96C97=CC=CC=C97C98=CC=CC=C98C99=CC=CC=C99C100=CC=CC=C100C101=CC=CC=C101C102=CC=CC=C102C103=CC=CC=C103C104=CC=CC=C104C105=CC=CC=C105C106=CC=CC=C106C107=CC=CC=C107C108=CC=CC=C108C109=CC=CC=C109C110=CC=CC=C110C111=CC=CC=C111C112=CC=CC=C112C113=CC=CC=C113C114=CC=CC=C114C115=CC=CC=C115C116=CC=CC=C116C117=CC=CC=C117C118=CC=CC=C118C119=CC=CC=C119C120=CC=CC=C120C121=CC=CC=C121C122=CC=CC=C122C123=CC=CC=C123C124=CC=CC=C124C125=CC=CC=C125C126=CC=CC=C126C127=CC=CC=C127C128=CC=CC=C128C129=CC=CC=C129C130=CC=CC=C130C131=CC=CC=C131C132=CC=CC=C132C133=CC=CC=C133C134=CC=CC=C134C135=CC=CC=C135C136=CC=CC=C136C137=CC=CC=C137C138=CC=CC=C138C139=CC=CC=C139C140=CC=CC=C140C141=CC=CC=C141C142=CC=CC=C142C143=CC=CC=C143C144=CC=CC=C144C145=CC=CC=C145C146=CC=CC=C146C147=CC=CC=C147C148=CC=CC=C148C149=CC=CC=C149C150=CC=CC=C150C151=CC=CC=C151C152=CC=CC=C152C153=CC=CC=C153C154=CC=CC=C154C155=CC=CC=C155C156=CC=CC=C156C157=CC=CC=C157C158=CC=CC=C158C159=CC=CC=C159C160=CC=CC=C160C161=CC=CC=C161C162=CC=CC=C162C163=CC=CC=C163C164=CC=CC=C164C165=CC=CC=C165C166=CC=CC=C166C167=CC=CC=C167C168=CC=CC=C168C169=CC=CC=C169C170=CC=CC=C170C171=CC=CC=C171C172=CC=CC=C172C173=CC=CC=C173C174=CC=CC=C174C175=CC=CC=C175C176=CC=CC=C176C177=CC=CC=C177C178=CC=CC=C178C179=CC=CC=C179C180=CC=CC=C180C181=CC=CC=C181C182=CC=CC=C182C183=CC=CC=C183C184=CC=CC=C184C185=CC=CC=C185C186=CC=CC=C186C187=CC=CC=C187C188=CC=CC=C188C189=CC=CC=C189C190=CC=CC=C190C191=CC=CC=C191C192=CC=CC=C192C193=CC=CC=C193C194=CC=CC=C194C195=CC=CC=C195C196=CC=CC=C196C197=CC=CC=C197C198=CC=CC=C198C199=CC=CC=C199C200=CC=CC=C200C201=CC=CC=C201C202=CC=CC=C202C203=CC=CC=C203C204=CC=CC=C204C205=CC=CC=C205C206=CC=CC=C206C207=CC=CC=C207C208=CC=CC=C208C209=CC=CC=C209C210=CC=CC=C210C211=CC=CC=C211C212=CC=CC=C212C213=CC=CC=C213C214=CC=CC=C214C215=CC=CC=C215C216=CC=CC=C216C217=CC=CC=C217C218=CC=CC=C218C219=CC=CC=C219C220=CC=CC=C220C221=CC=CC=C221C222=CC=CC=C222C223=CC=CC=C223C224=CC=CC=C224C225=CC=CC=C225C226=CC=CC=C226C227=CC=CC=C227C228=CC=CC=C228C229=CC=CC=C229C230=CC=CC=C230C231=CC=CC=C231C232=CC=CC=C232C233=CC=CC=C233C234=CC=CC=C234C235=CC=CC=C235C236=CC=CC=C236C237=CC=CC=C237C238=CC=CC=C238C239=CC=CC=C239C240=CC=CC=C240C241=CC=CC=C241C242=CC=CC=C242C243=CC=CC=C243C244=CC=CC=C244C245=CC=CC=C245C246=CC=CC=C246C247=CC=CC=C247C248=CC=CC=C248C249=CC=CC=C249C250=CC=CC=C250C251=CC=CC=C251C252=CC=CC=C252C253=CC=CC=C253C254=CC=CC=C254C255=CC=CC=C255C256=CC=CC=C256C257=CC=CC=C257C258=CC=CC=C258C259=CC=CC=C259C260=CC=CC=C260C261=CC=CC=C261C262=CC=CC=C262C263=CC=CC=C263C264=CC=CC=C264C265=CC=CC=C265C266=CC=CC=C266C267=CC=CC=C267C268=CC=CC=C268C269=CC=CC=C269C270=CC=CC=C270C271=CC=CC=C271C272=CC=CC=C272C273=CC=CC=C273C274=CC=CC=C274C275=CC=CC=C275C276=CC=CC=C276C277=CC=CC=C277C278=CC=CC=C278C279=CC=CC=C279C280=CC=CC=C280C281=CC=CC=C281C282=CC=CC=C282C283=CC=CC=C283C284=CC=CC=C284C285=CC=CC=C285C286=CC=CC=C286C287=CC=CC=C287C288=CC=CC=C288C289=CC=CC=C289C290=CC=CC=C290C291=CC=CC=C291C292=CC=CC=C292C293=CC=CC=C293C294=CC=CC=C294C295=CC=CC=C295C296=CC=CC=C296C297=CC=CC=C297C298=CC=CC=C298C299=CC=CC=C299C300=CC=CC=C300C301=CC=CC=C301C302=CC=CC=C302C303=CC=CC=C303C304=CC=CC=C304C305=CC=CC=C305C306=CC=CC=C306C307=CC=CC=C307C308=CC=CC=C308C309=CC=CC=C309C310=CC=CC=C310C311=CC=CC=C311C312=CC=CC=C312C313=CC=CC=C313C314=CC=CC=C314C315=CC=CC=C315C316=CC=CC=C316C317=CC=CC=C317C318=CC=CC=C318C319=CC=CC=C319C320=CC=CC=C320C321=CC=CC=C321C322=CC=CC=C322C323=CC=CC=C323C324=CC=CC=C324C325=CC=CC=C325C326=CC=CC=C326C327=CC=CC=C327C328=CC=CC=C328C329=CC=CC=C329C330=CC=CC=C330C331=CC=CC=C331C332=CC=CC=C332C333=CC=CC=C333C334=CC=CC=C334C335=CC=CC=C335C336=CC=CC=C336C337=CC=CC=C337C338=CC=CC=C338C339=CC=CC=C339C340=CC=CC=C340C341=CC=CC=C341C342=CC=CC=C342C343=CC=CC=C343C344=CC=CC=C344C345=CC=CC=C345C346=CC=CC=C346C347=CC=CC=C347C348=CC=CC=C348C349=CC=CC=C349C350=CC=CC=C350C351=CC=CC=C351C352=CC=CC=C352C353=CC=CC=C353C354=CC=CC=C354C355=CC=CC=C355C356=CC=CC=C356C357=CC=CC=C357C358=CC=CC=C358C359=CC=CC=C359C360

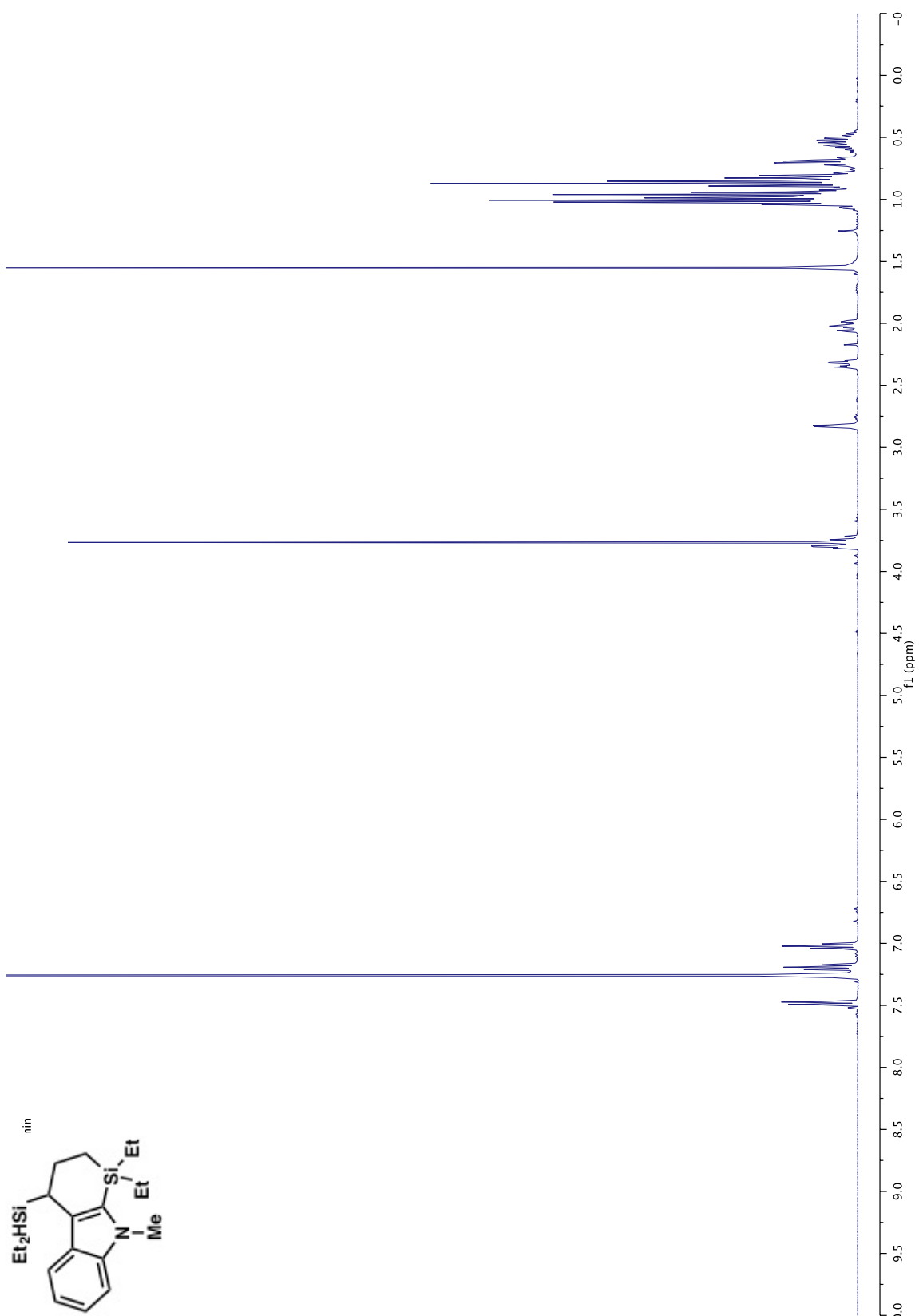


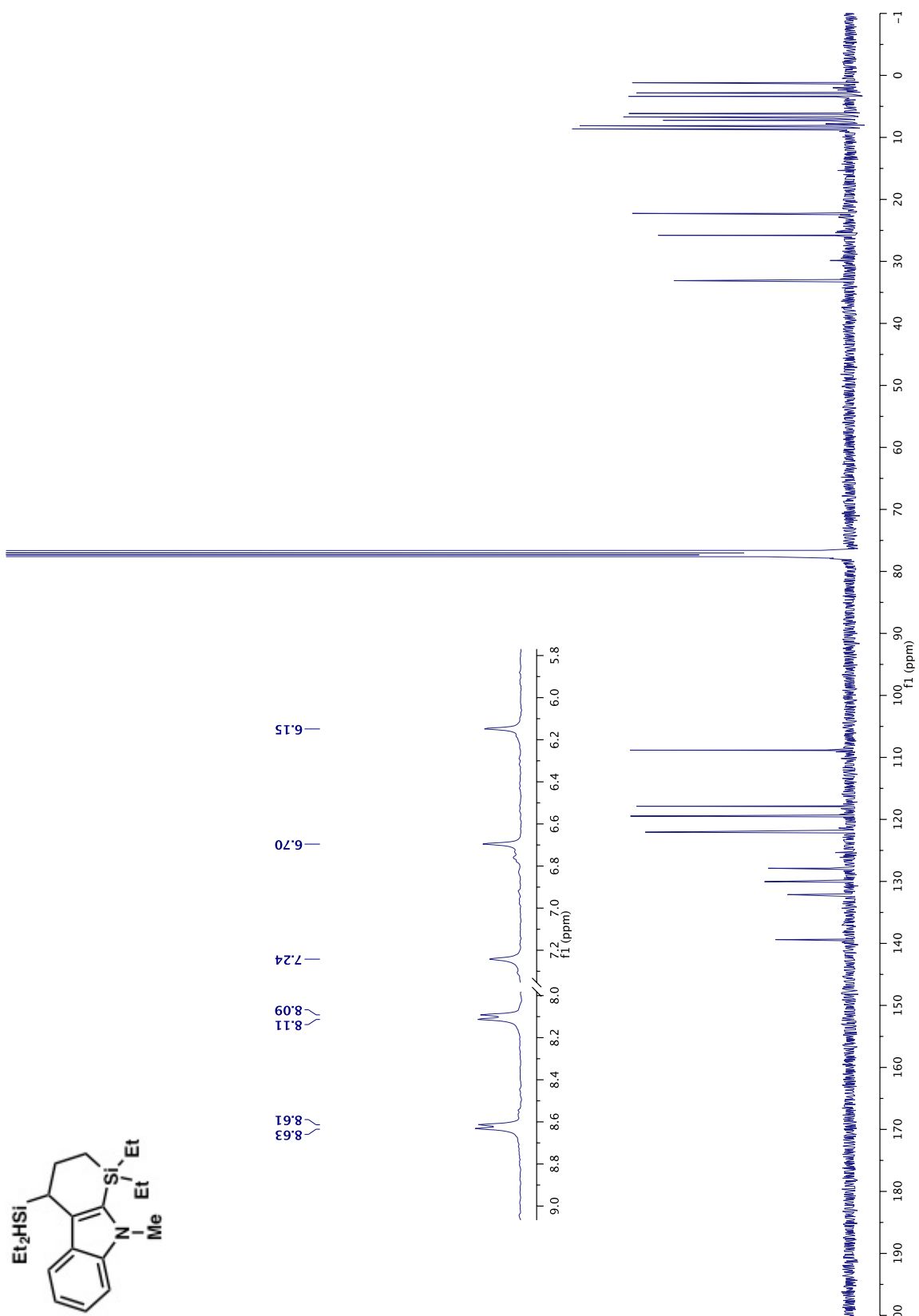


COSY (400 MHz, CDCl₃) of compound **9**.

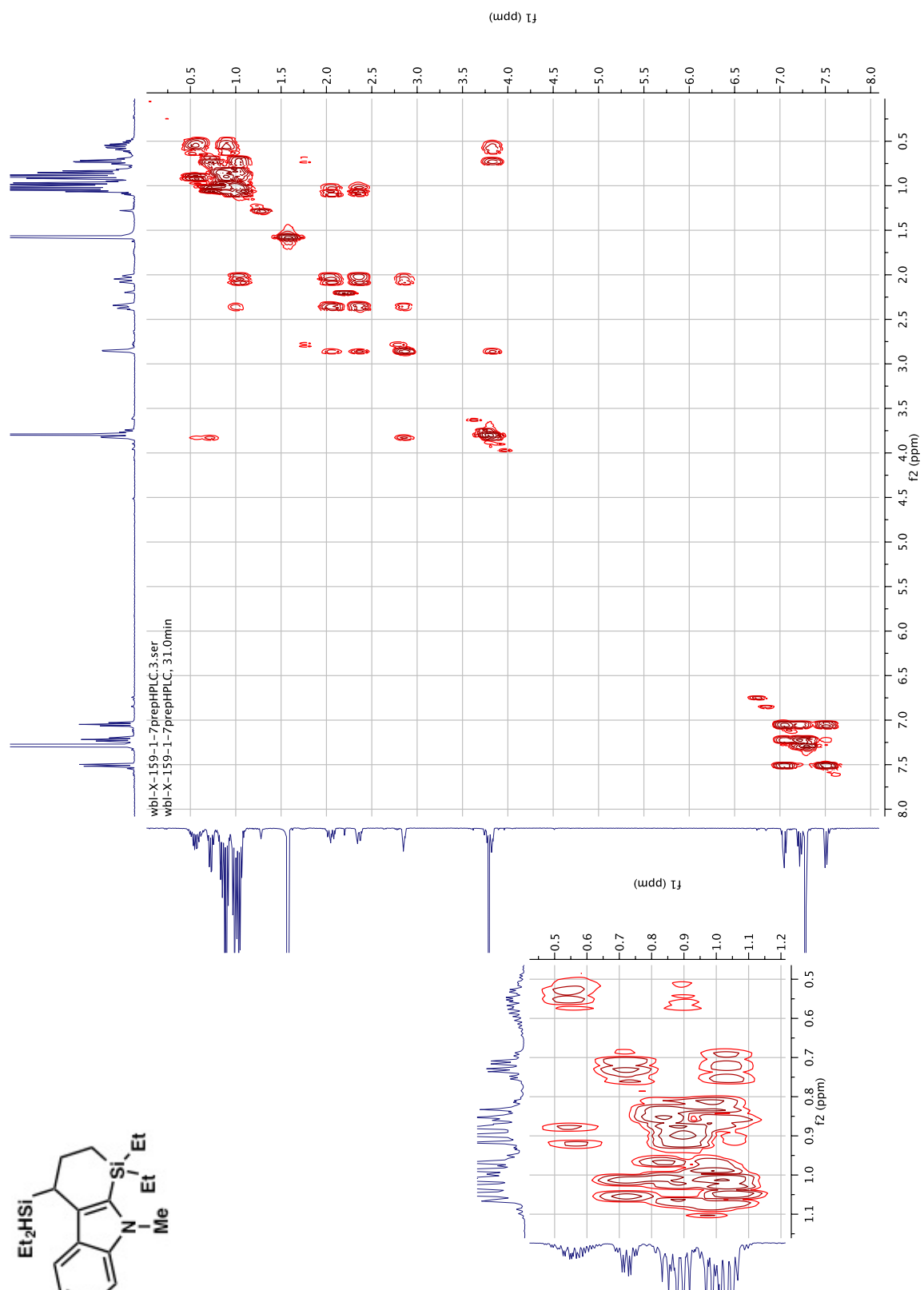


HSQC (400 MHz, CDCl₃) of compound **9**.

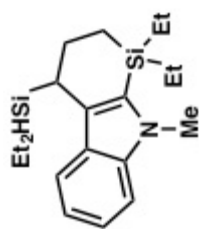
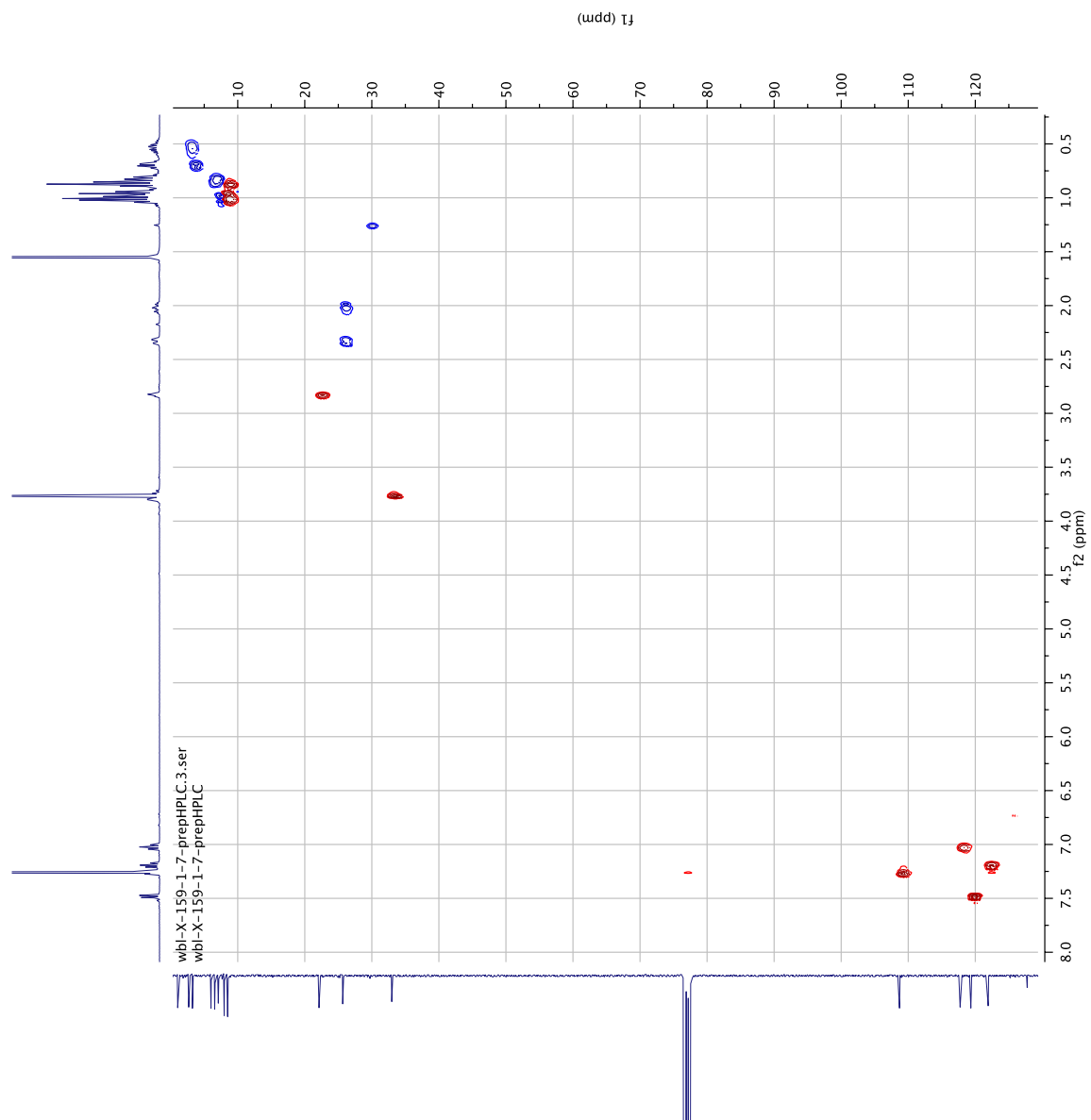


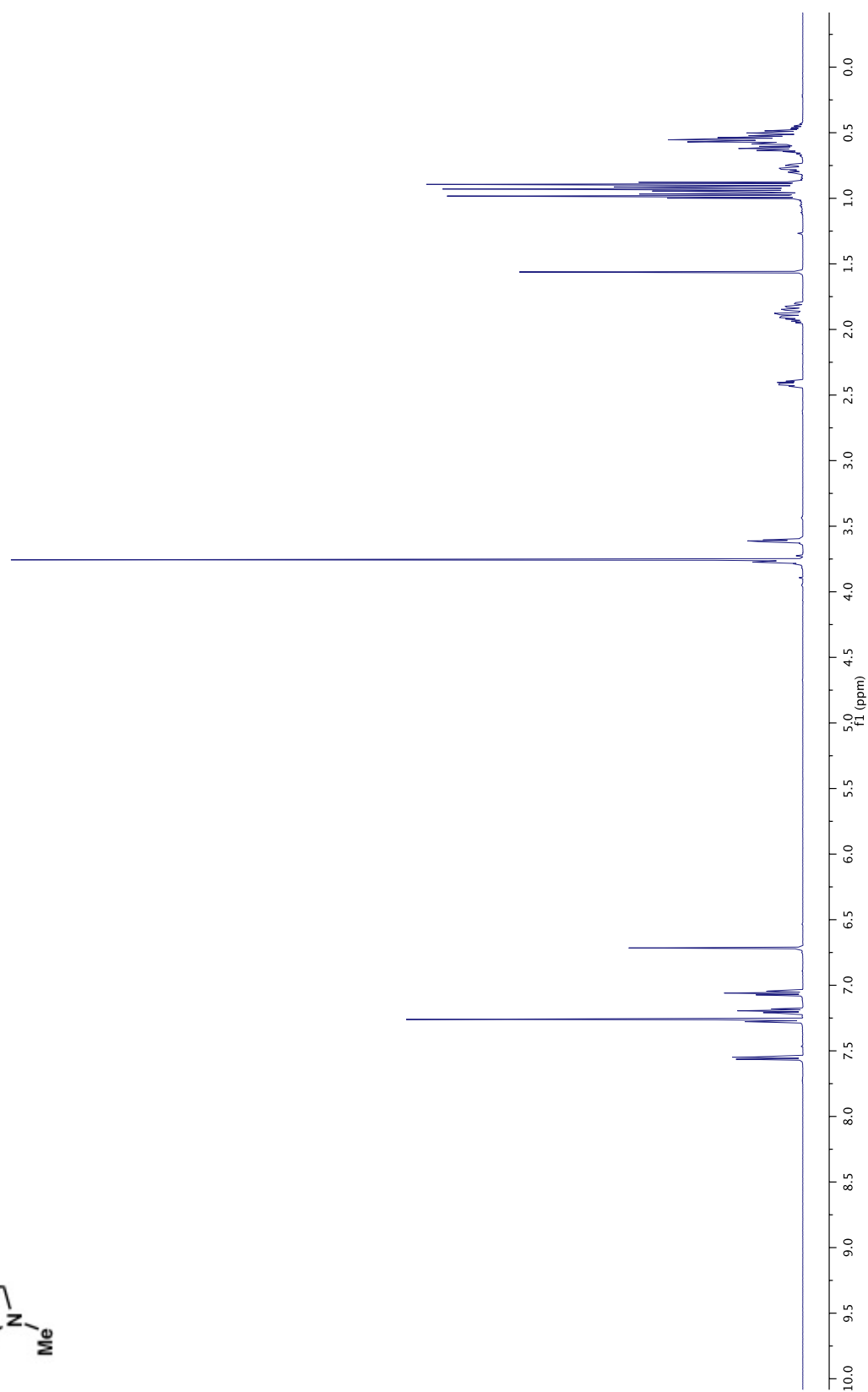
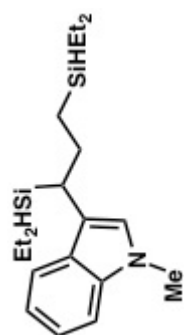


¹³C NMR (100 MHz, CDCl₃) of compound **10**.

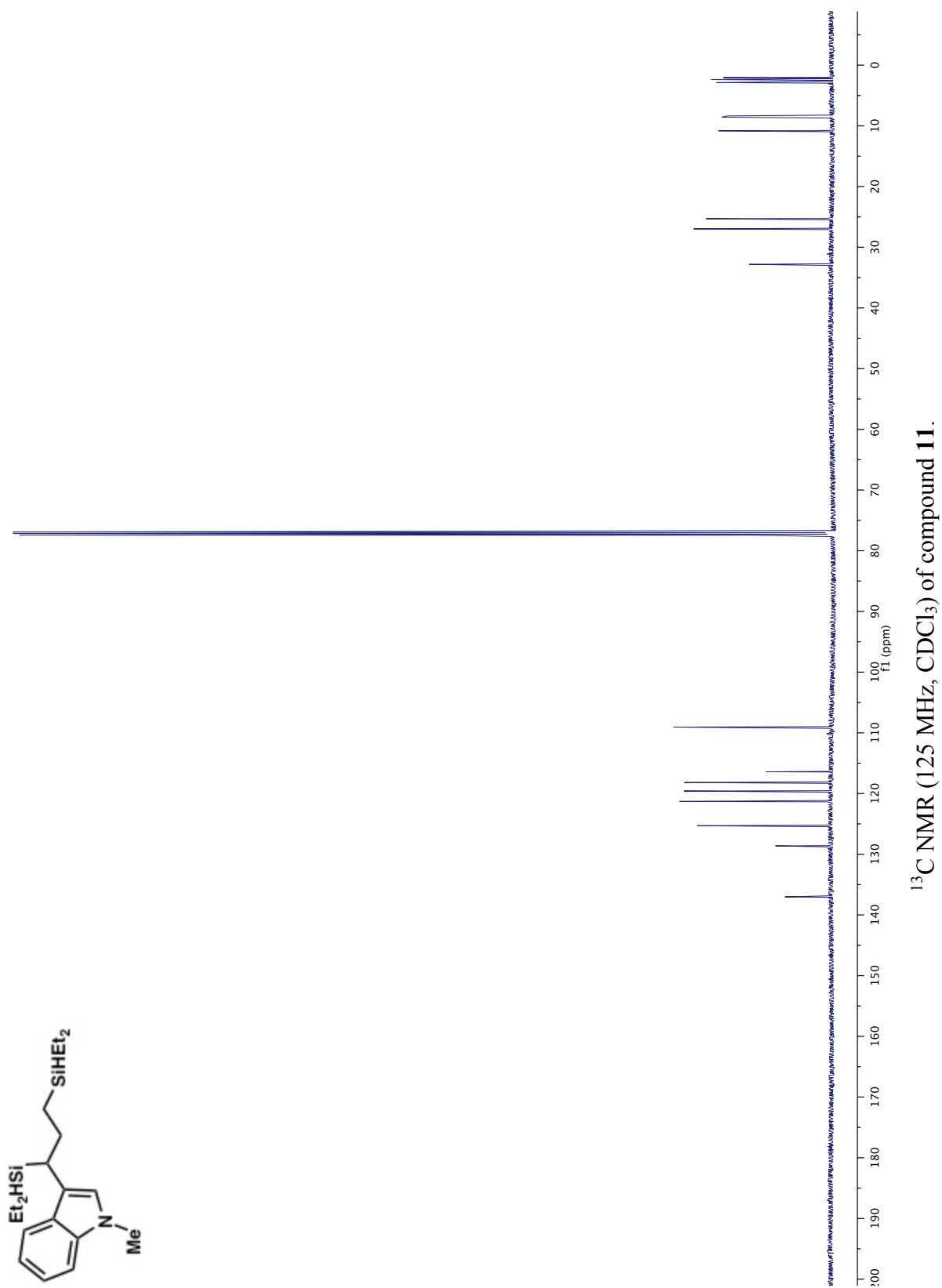


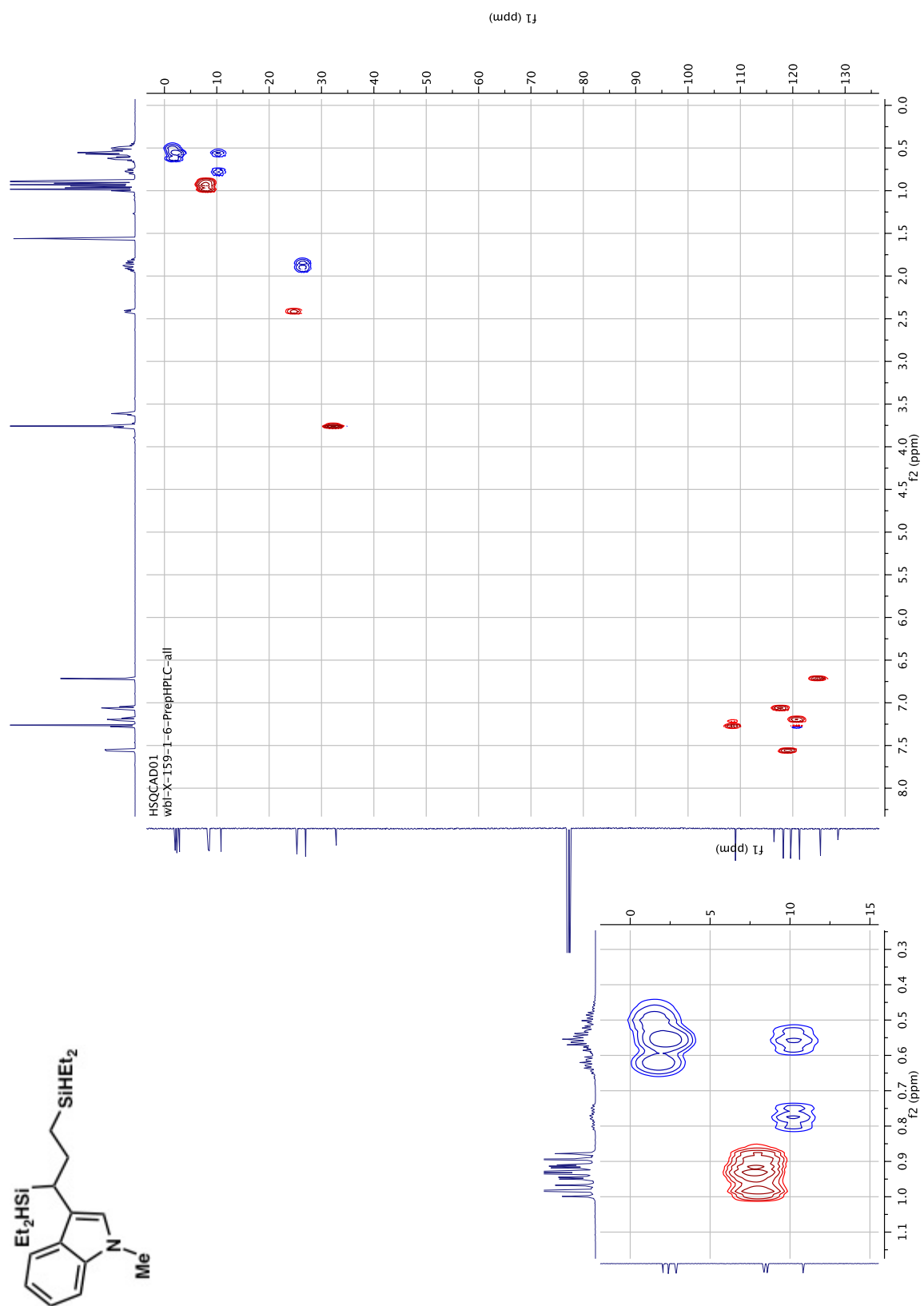
COSY (400 MHz, CDCl₃) of compound **10**.



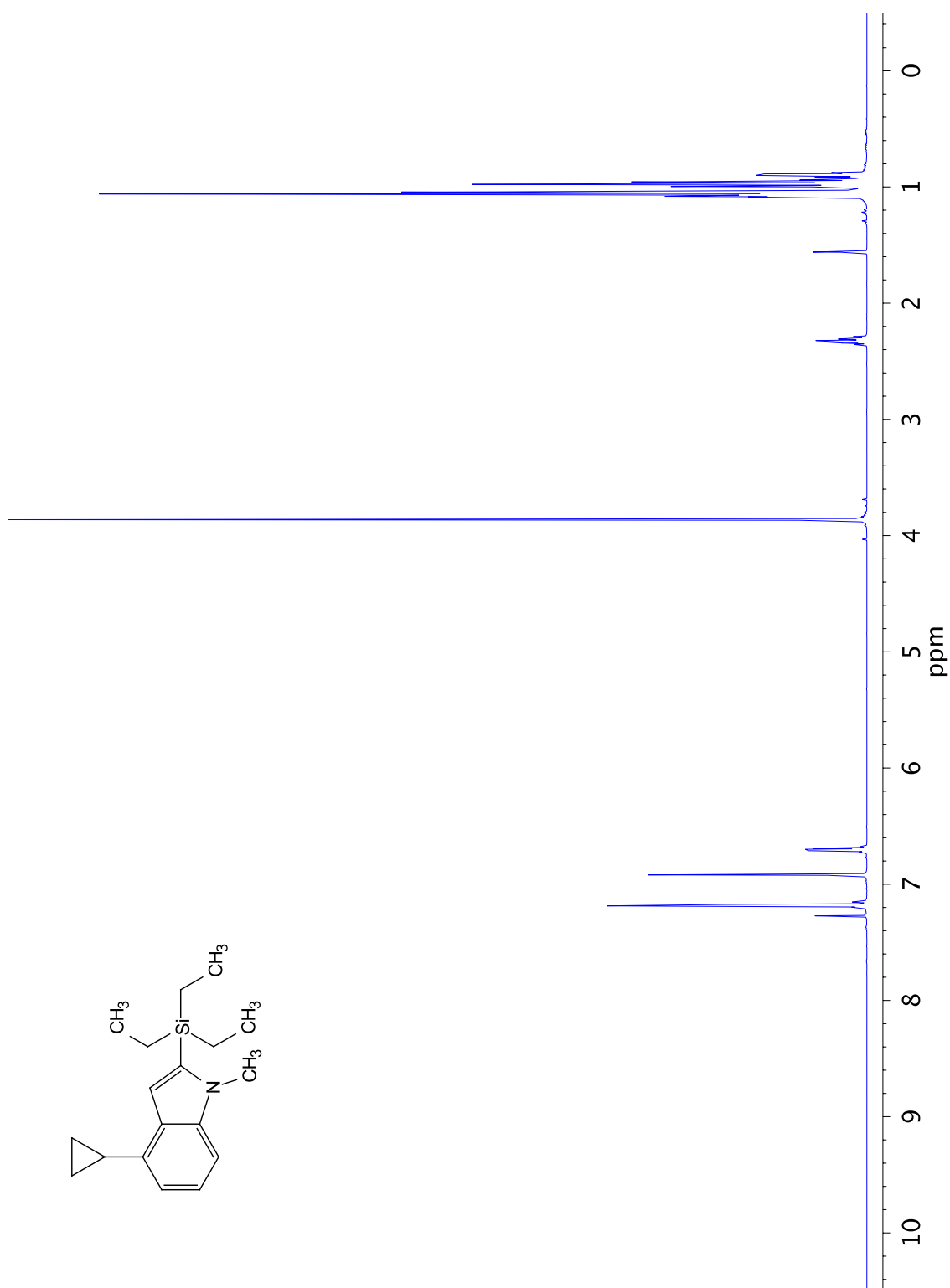


^1H NMR (500 MHz, CDCl_3) of compound **11**.

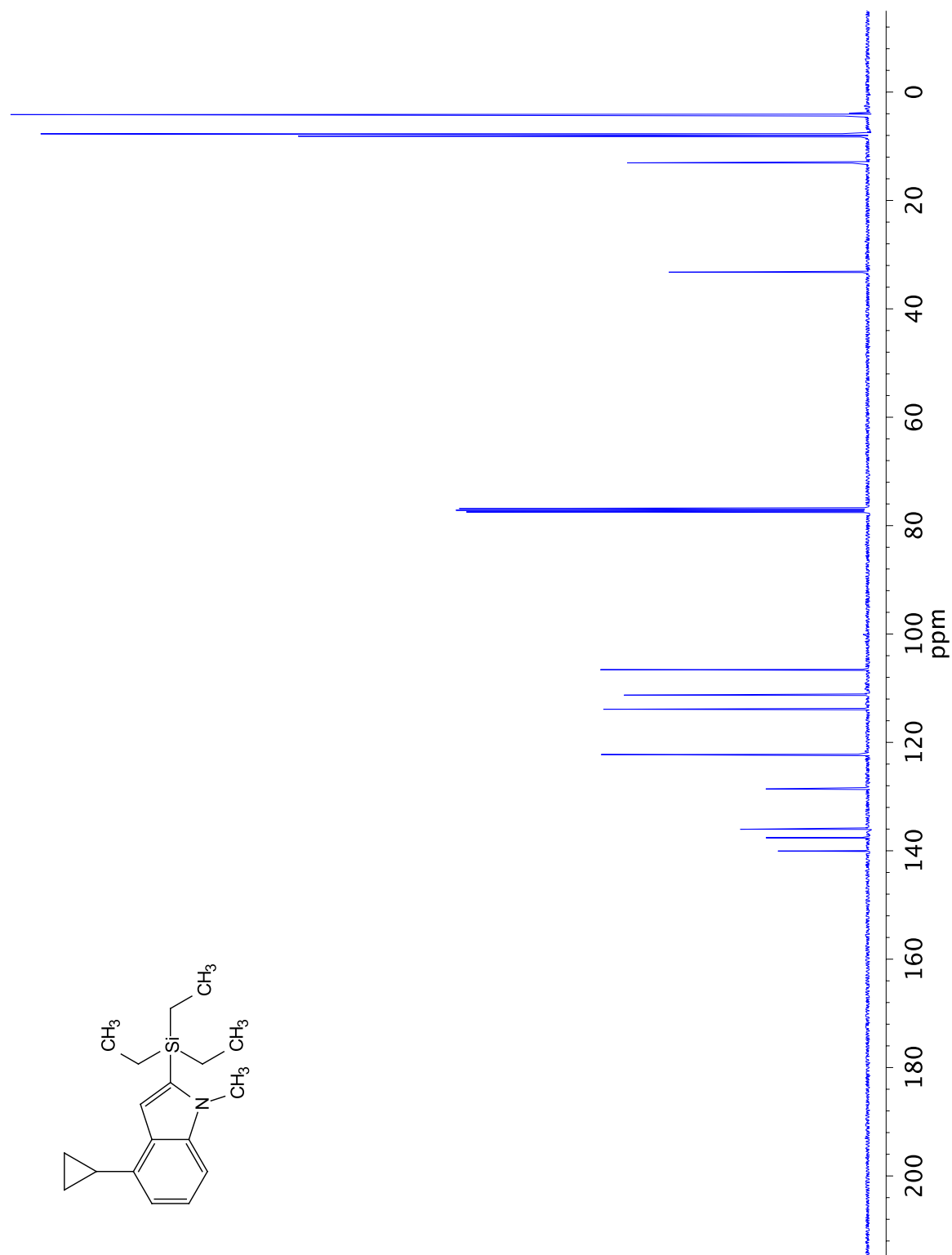


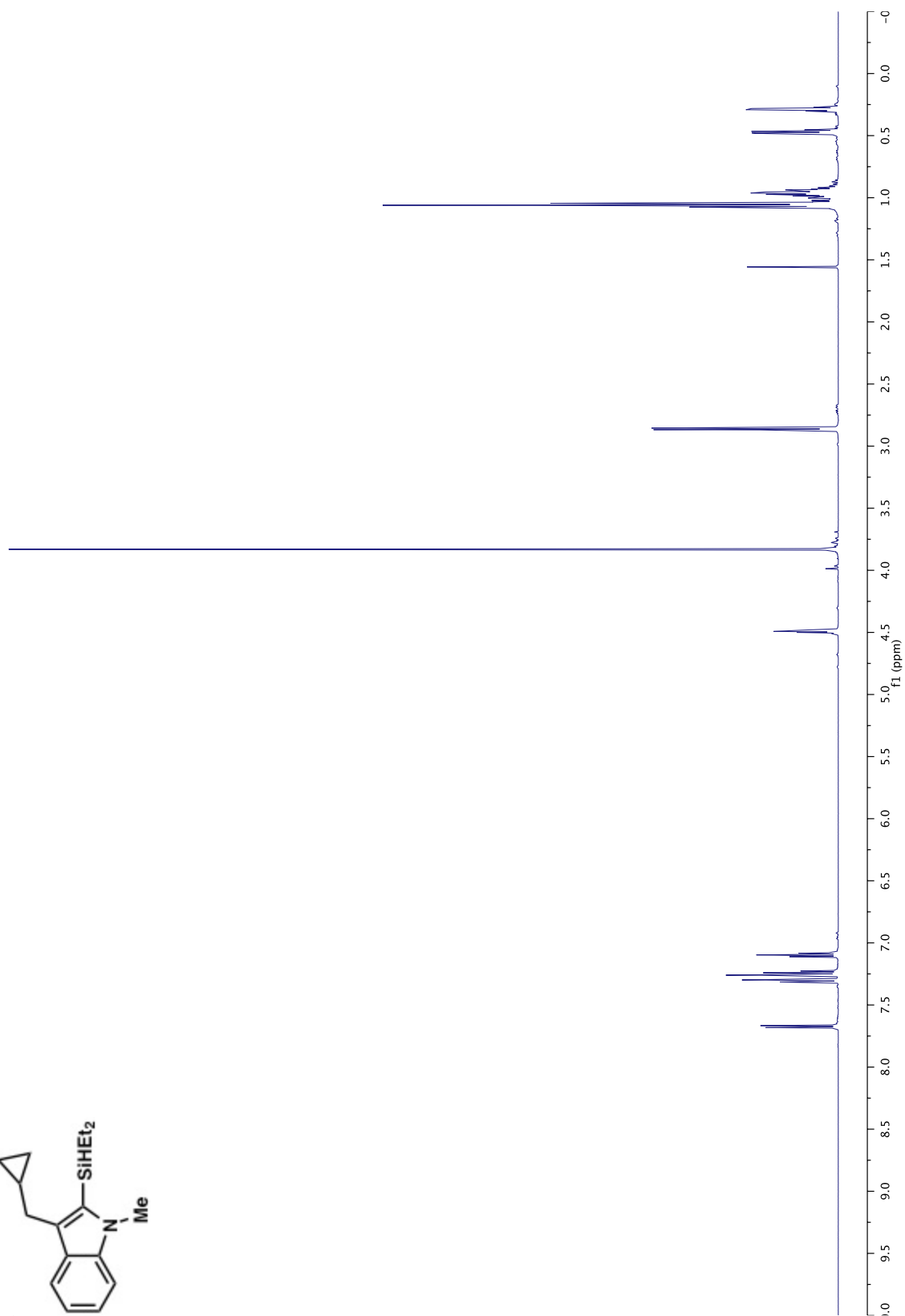
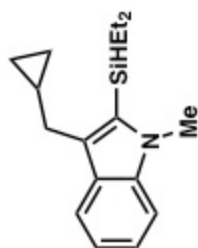


HSQC (500 MHz, CDCl₃) of compound **11**.

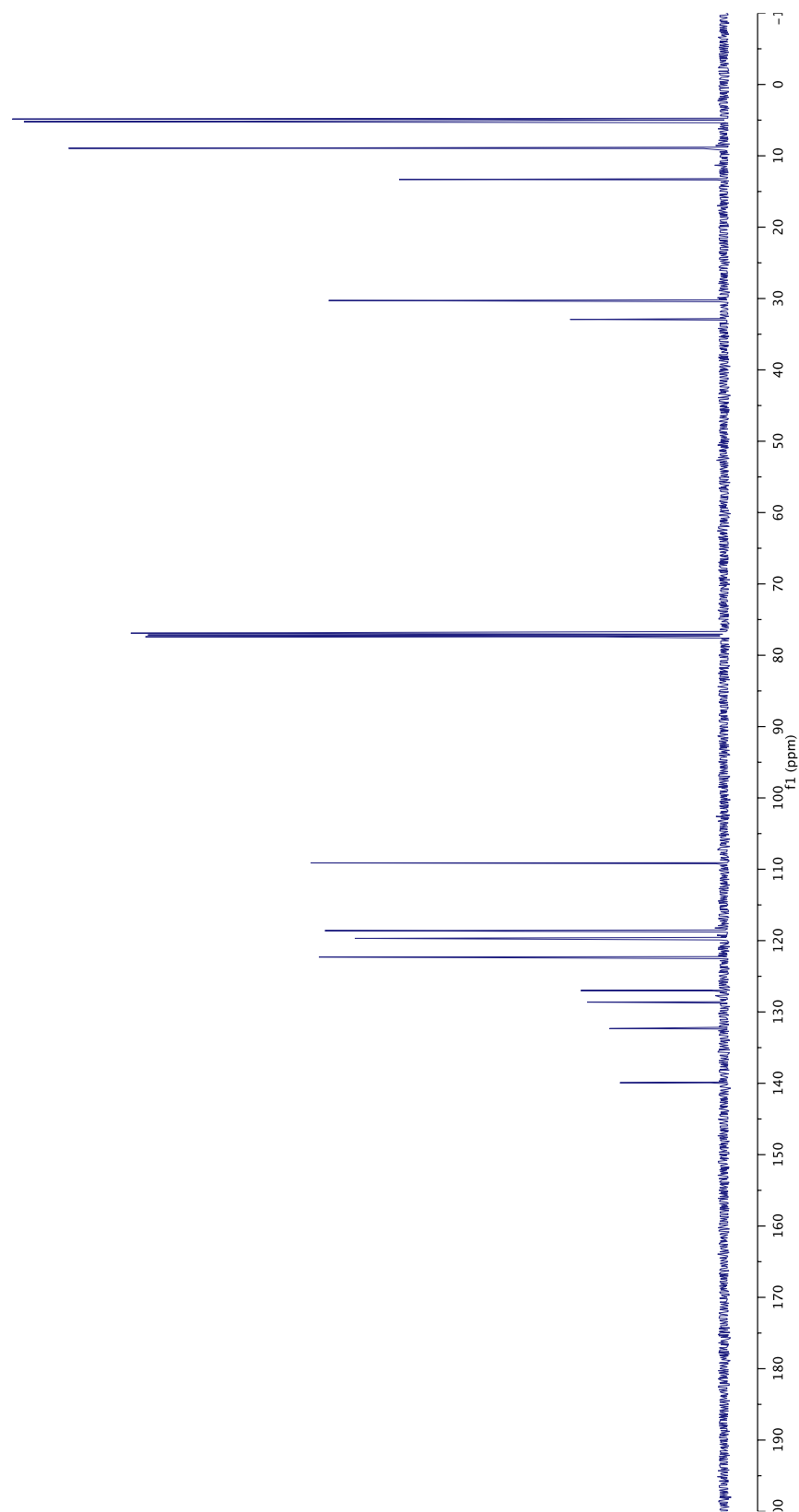
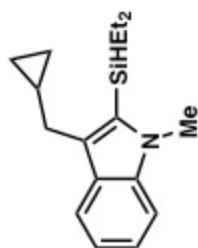


¹H NMR (500 MHz, CDCl₃) of compound **12**.

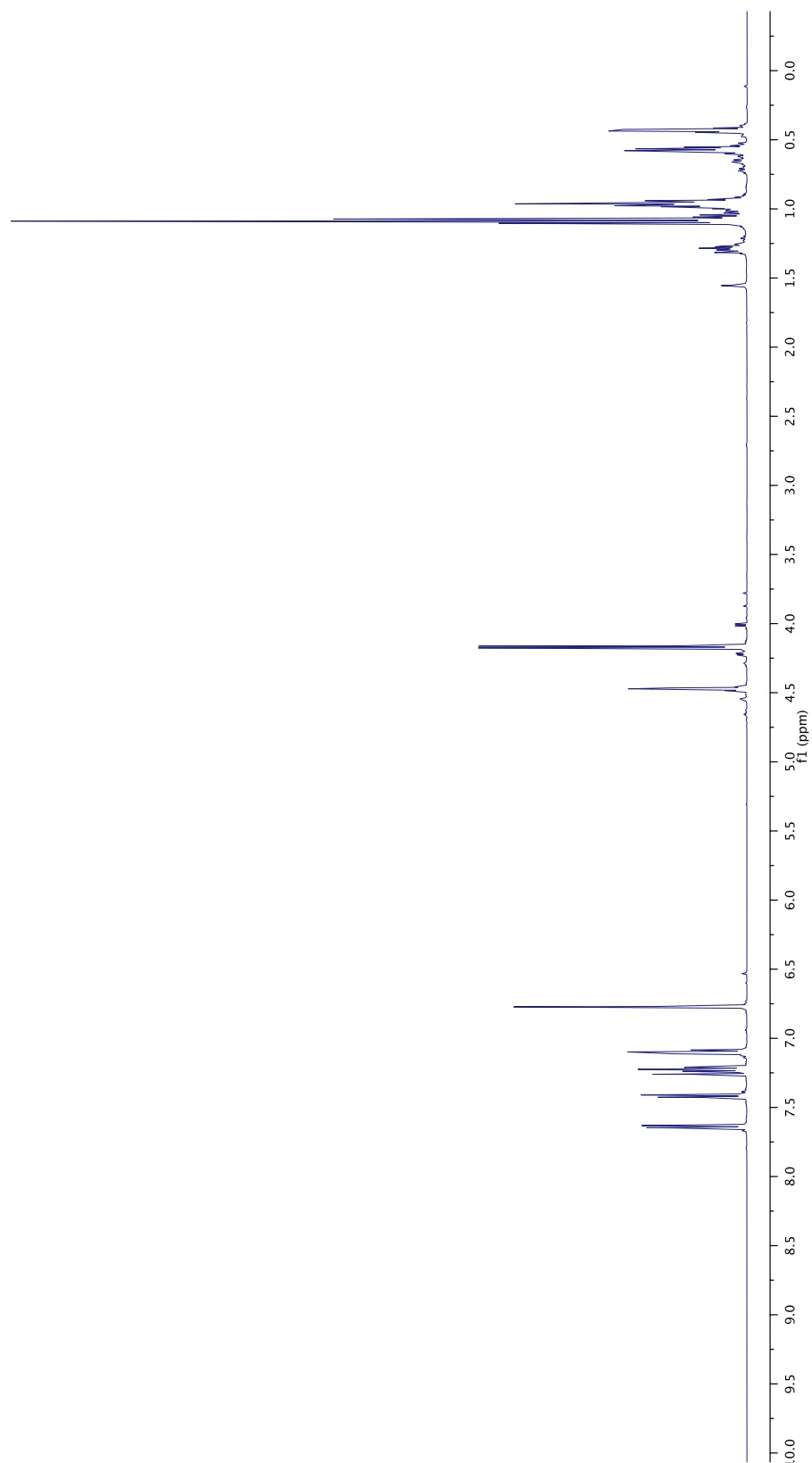
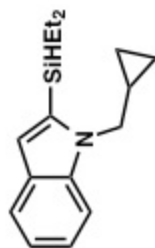




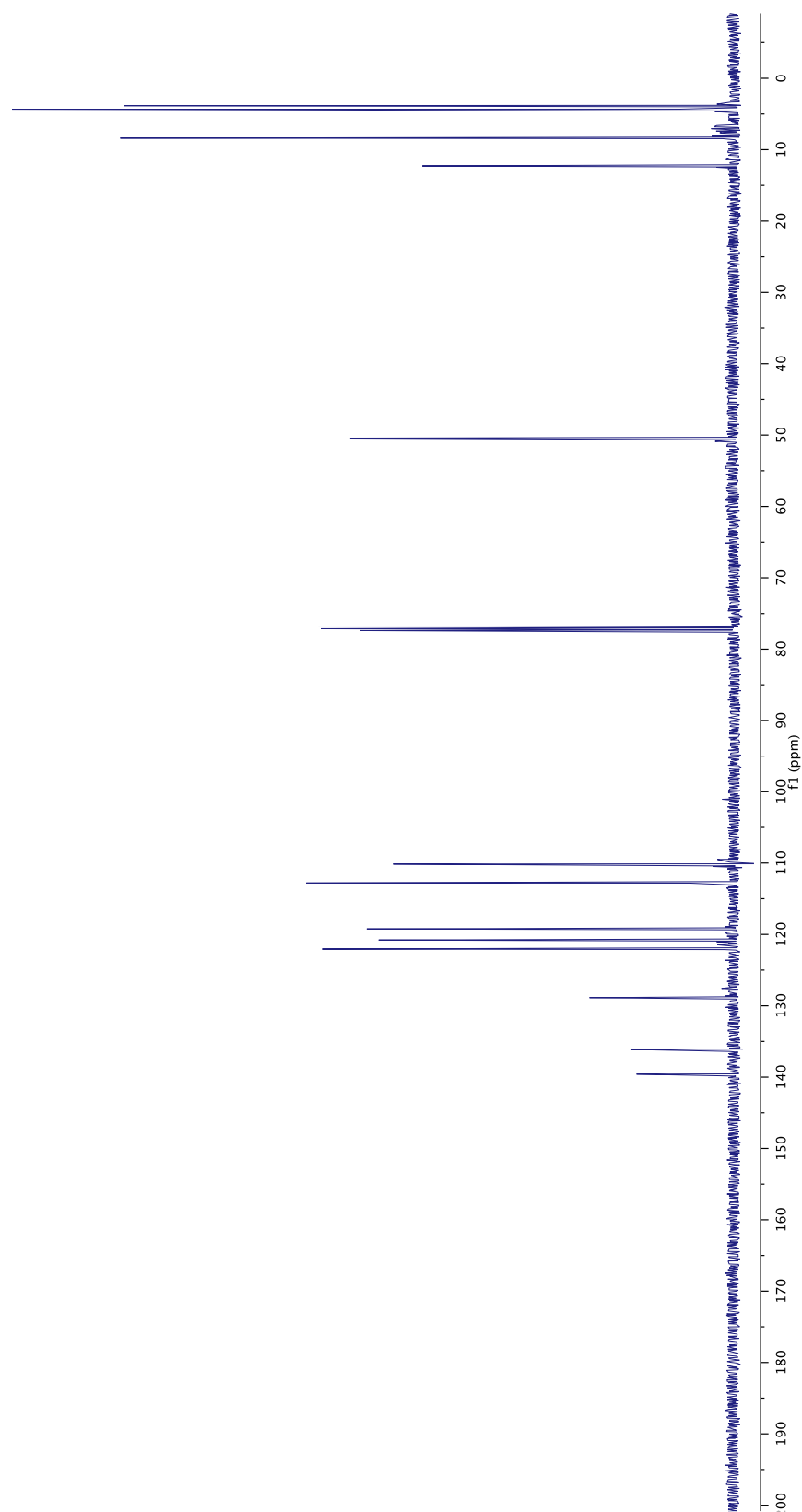
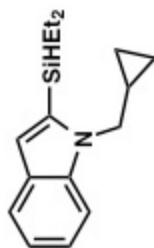
^1H NMR (500 MHz, CDCl_3) of compound **13**.



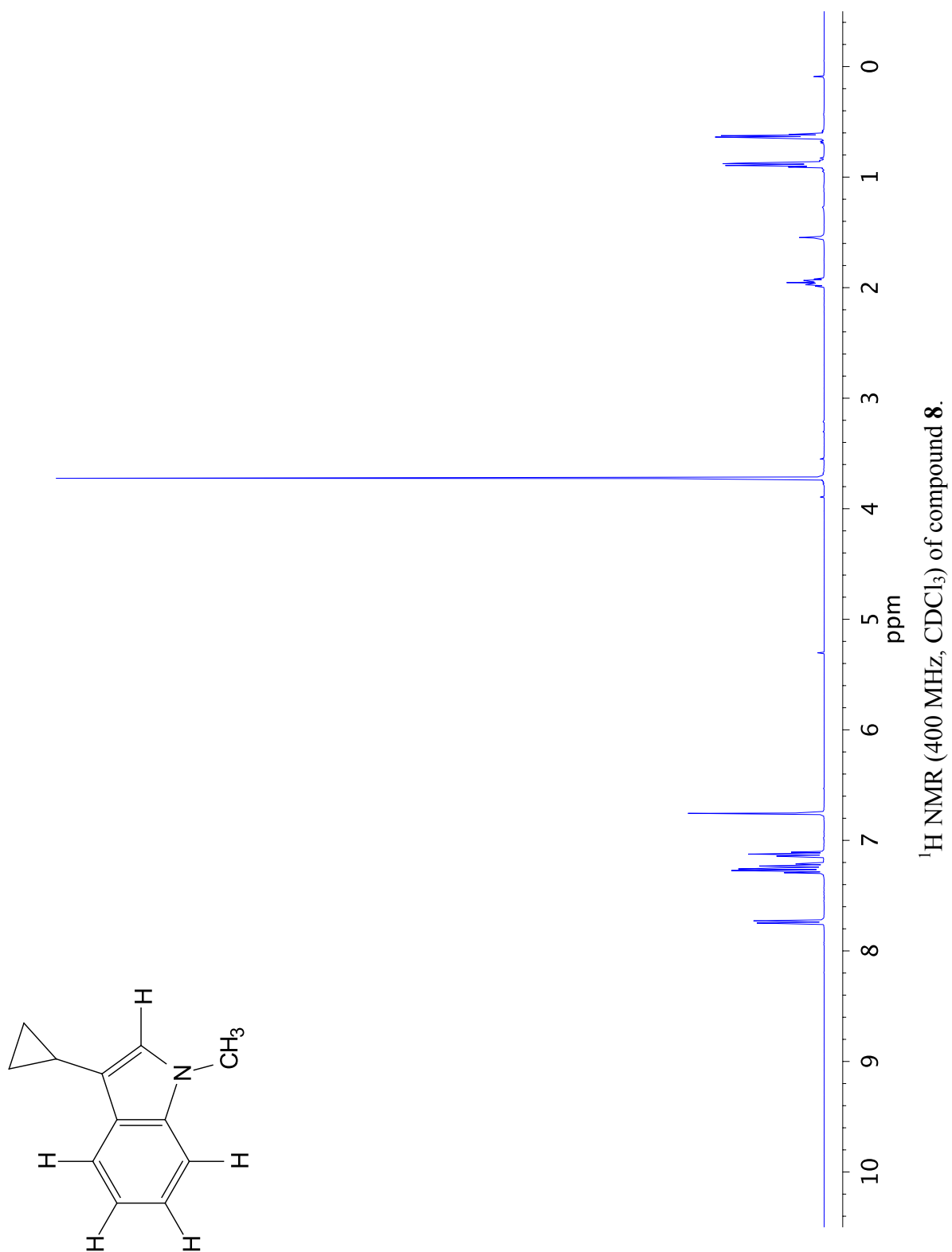
^{13}C NMR (125 MHz, CDCl_3) of compound **13**.

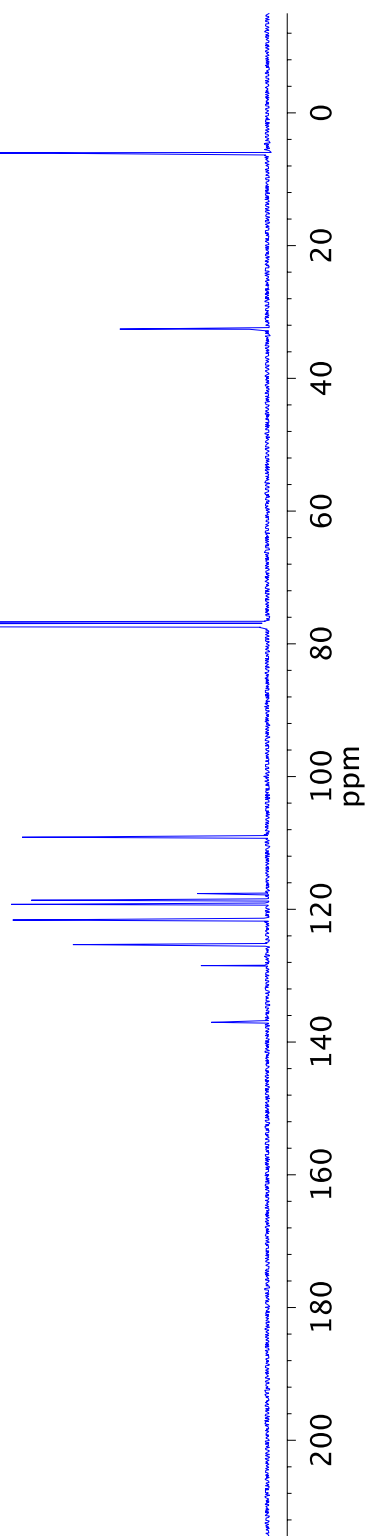
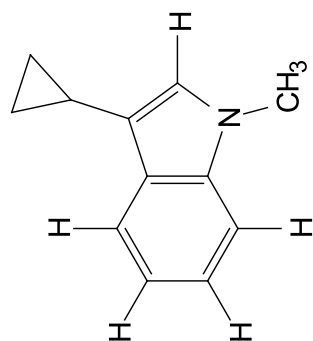


^1H NMR (500 MHz, CDCl_3) of compound **14**.

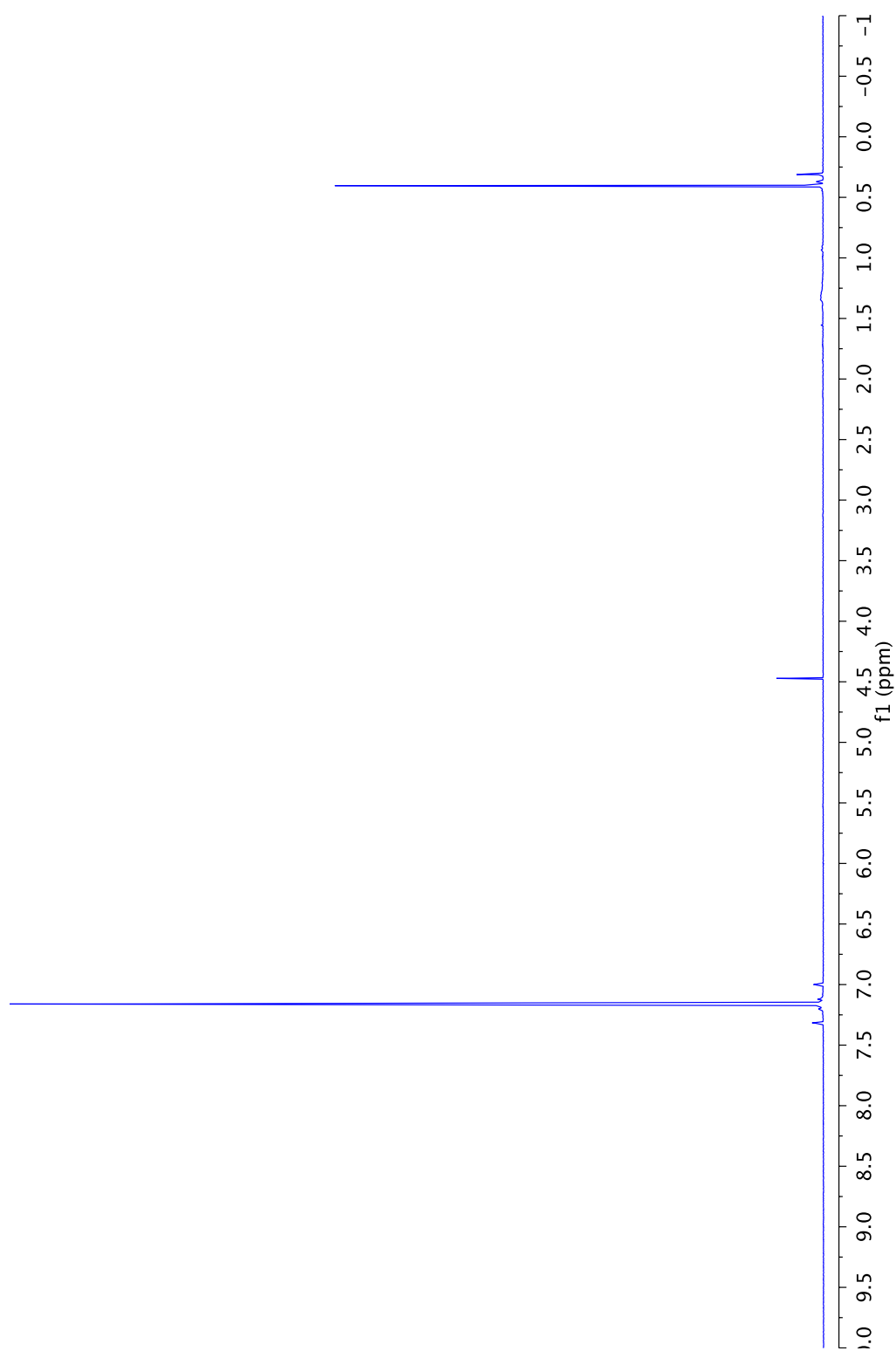


^{13}C NMR (125 MHz, CDCl_3) of compound 14.

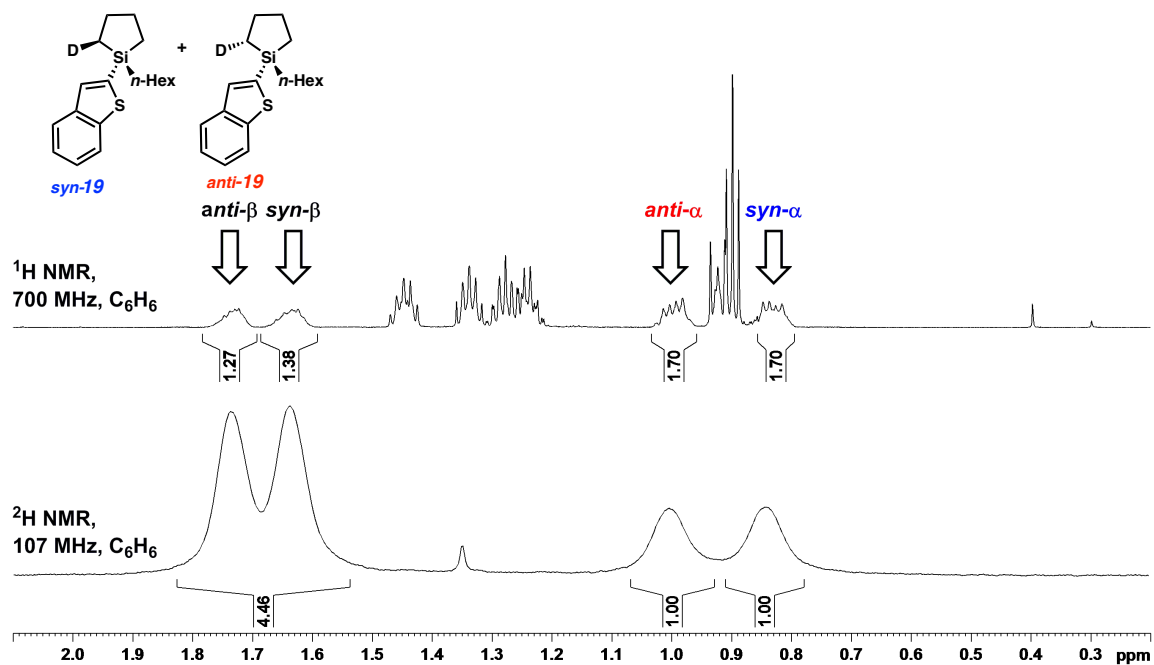
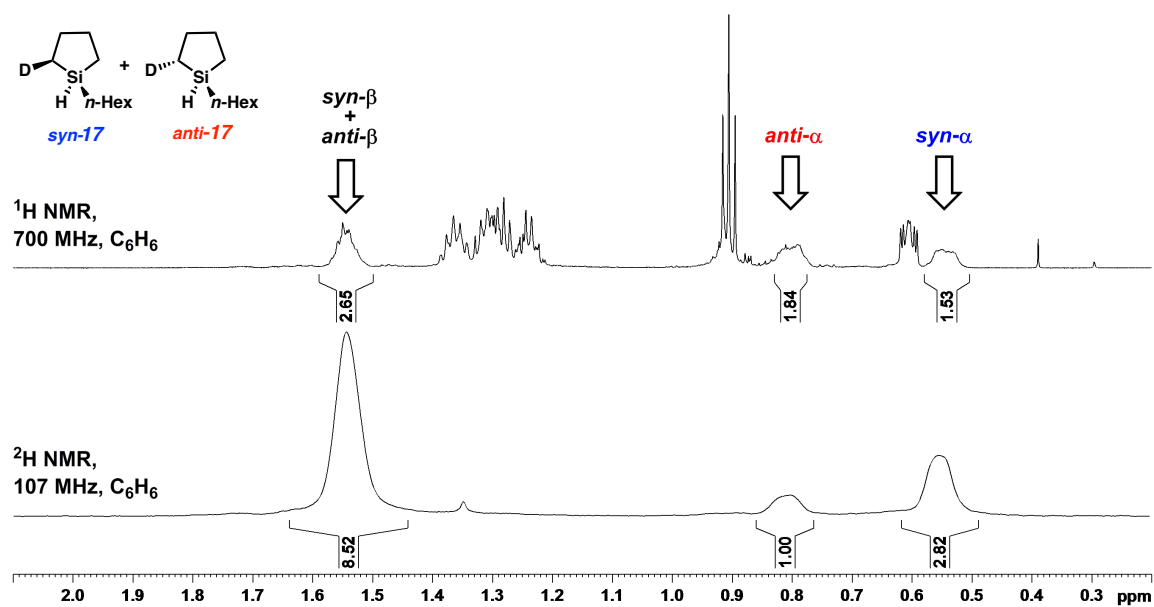




¹³C NMR (101 MHz, CDCl₃) of compound **8**.



^1H NMR (400 MHz, CDCl_3) of headspace gas for Figure 3.



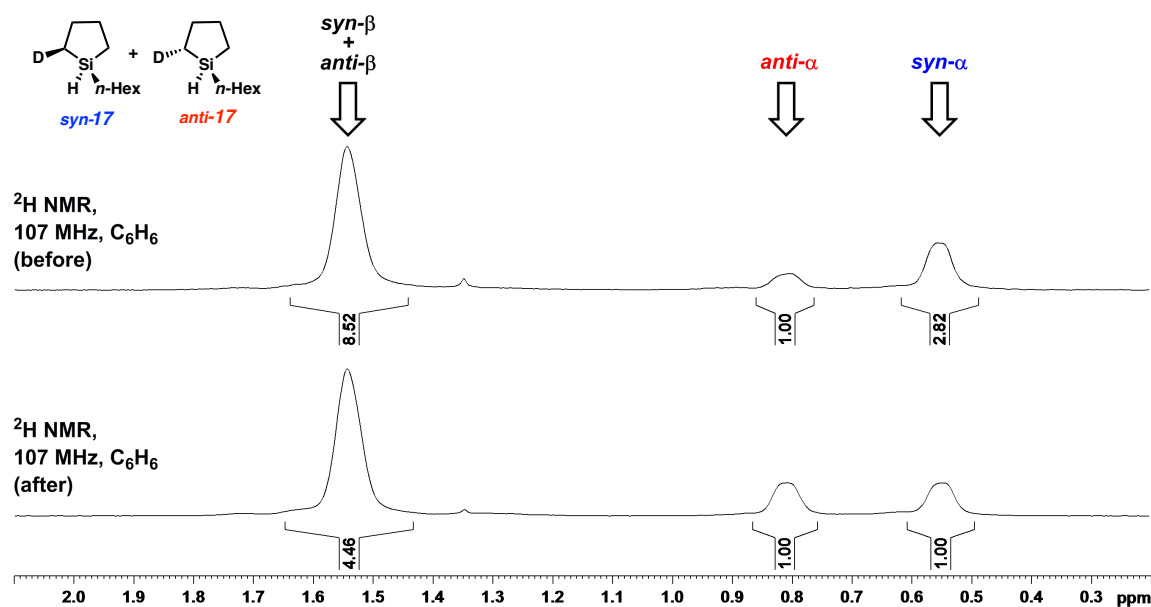


Figure 24. ^1H and ^2H NMR spectra of 1-(benzo[*b*]thiophen-2-yl)-1-hexylsilolane: scrambling of the configuration at the silicon atom.

Zero-point correction (ZPE), thermal correction to energy (ΔE), thermal correction to enthalpy (ΔH), thermal correction to Gibbs free energy (ΔG), energies (E), enthalpies (H), and Gibbs free energies (G) (in Hartree) of the structures calculated at the M062X/6-311+G(d,p)-CPCM(THF)//B3LYP/6-31G(d) level of theory. The radical species were calculated at the UM062X/6-311+G(d,p)-CPCM(THF)//UB3LYP/6-31G(d) level of theory.

Table S1.

Structures	ZPE	ΔE	ΔH	ΔG	E	H	G	Imaginary Frequency (cm^{-1})
KOtBu	0.123876	0.13225	0.133194	0.089516	-833.005741	-832.872547	-832.916225	—
[KOtBu] ₂	0.248731	0.267161	0.268105	0.197204	-1666.044513	-1665.776408	-1665.847309	—
[KOtBu] ₃	0.373819	0.402210	0.403154	0.308232	-2499.076483	-2498.673329	-2498.768251	—
[KOtBu] ₄	0.498948	0.537092	0.538036	0.423883	-3332.132729	-3331.594693	-3331.708846	—
NaOtBu	0.124504	0.132747	0.133691	0.091144	-395.346359	-395.212668	-395.255215	—
[NaOtBu] ₂	0.250728	0.268441	0.269385	0.201573	-790.735054	-790.465669	-790.533481	—
[NaOtBu] ₃	0.376694	0.404037	0.404981	0.314435	-1186.1147	-1185.709722	-1185.800268	—
[NaOtBu] ₄	0.503381	0.539676	0.540621	0.432343	-1581.528698	-1580.988077	-1581.096355	—
[KOtBu] ₃ K ⁺	0.376381	0.405929	0.406873	0.313063	-3098.96526	-3098.558385	-3098.652195	—
tBuO [•]	0.120285	0.126780	0.127724	0.091493	-233.106915	-232.979191	-233.015422	—
K ⁺	0.000000	0.001416	0.00236	-0.015176	-599.852623	-599.850263	-599.867799	—
O ₂	0.003779	0.006142	0.007086	-0.016200	-150.307709	-150.300623	-150.323909	—
HSiMe ₃	0.119775	0.127259	0.128203	0.089443	-409.808109	-409.679906	-409.718666	—

Me3Si ⁺	0.110424	0.117885	0.118829	0.079221	-409.158688	-409.039859	-409.079467	—
H ⁺	0.000000	0.001416	0.002360	-0.010654	-0.498155	-0.495795	-0.508809	—
H2	0.010145	0.012505	0.013450	-0.001342	-1.168439	-1.154989	-1.169781	—
Me ⁺	0.029833	0.032939	0.033883	0.011043	-39.821500	-39.787617	-39.810457	—
tBuO ⁺	0.123045	0.129569	0.130513	0.093490	-232.959433	-232.828920	-232.865943	—
tBuOH	0.136186	0.142910	0.143854	0.107187	-233.635990	-233.492136	-233.528803	—
tBuOSiMe3	0.239087	0.253167	0.254111	0.199885	-642.300631	-642.046520	-642.100746	—
TS1	0.240733	0.255166	0.256110	0.199354	-642.763935	-642.507825	-642.564581	-1030.485
KOO ⁺	0.004256	0.007861	0.008805	-0.022582	-750.315795	-750.306990	-750.338377	—
[KOtBu]KOO ⁺	0.129373	0.142803	0.143747	0.086220	-1583.351420	-1583.207673	-1583.265200	—
[KOtBu]3KOO ⁺ (C-2)	0.379600	0.412799	0.413743	0.311278	-3249.440807	-3249.027064	-3249.129529	—
NaOO ⁺	0.004544	0.007996	0.008940	-0.021306	-312.653761	-312.644821	-312.675067	—
[NaOtBu]NaOO ⁺	0.130868	0.143717	0.144661	0.089114	-708.032569	-707.887908	-707.943455	—
[NaOtBu]3NaOO ⁺ (C-3)	0.383031	0.414968	0.415912	0.314971	-1498.821038	-1498.405126	-1498.506067	—
[KOtBu]HSiMe3	0.245120	0.262483	0.263428	0.197306	-1242.817802	-1242.554374	-1242.620496	—
TS29	0.121915	0.132160	0.133104	0.086788	-560.046427	-559.913323	-559.959639	-943.169
HOO ⁺	0.014028	0.016885	0.017829	-0.008164	-150.895667	-150.877838	-150.903831	—
[tBuOSiHMe3] ⁺	0.243120	0.257862	0.258806	0.203152	-642.926999	-642.668193	-642.723847	—
[tBuOSiMe3] ⁺⁺	0.233611	0.248473	0.249417	0.192055	-642.295269	-642.045852	-642.103214	—
[tBuOSiMe3][K ⁺	0.239438	0.255819	0.256763	0.193442	-1242.210702	-1241.953939	-1242.017260	—
N-Me-Indole (I)	0.157986	0.166006	0.166950	0.124908	-403.061521	-402.894571	-402.936613	—
TS-2	0.268329	0.284870	0.285814	0.222742	-812.217393	-811.931579	-811.994651	-253.094
TS-3	0.267908	0.284619	0.285563	0.221708	-812.212867	-811.927304	-811.991159	-300.146
C-5	0.268657	0.285198	0.286142	0.223901	-812.246530	-811.960388	-812.022629	—
C-6	0.268799	0.285357	0.286301	0.224289	-812.241640	-811.955339	-812.017351	—
TS-8	0.764863	0.820531	0.821475	0.668871	-4144.369894	-4143.548419	-4143.701023	-1121.184
TS-9	0.765361	0.820865	0.821809	0.669650	-4144.362660	-4143.540851	-4143.693010	-1225.729
C-10	0.260259	0.276207	0.277151	0.217055	-811.697822	-811.420671	-811.480767	—
C-11	0.260073	0.276139	0.277083	0.216367	-811.700813	-811.423730	-811.484446	—
C-9	0.512625	0.550863	0.551807	0.436236	-3332.668520	-3332.116713	-3332.232284	—
C-12	0.110675	0.116254	0.117198	0.081661	-249.437401	-249.320203	-249.355740	—
TS-10	0.221151	0.235065	0.236009	0.179441	-658.591231	-658.355222	-658.411790	-264.932
TS-11	0.220598	0.234647	0.235591	0.178681	-658.583048	-658.347457	-658.404367	-331.395
C-13	0.221494	0.235260	0.236205	0.181283	-658.615251	-658.379046	-658.433968	—
C-14	0.221193	0.235214	0.236158	0.180305	-658.604356	-658.368198	-658.424051	—
TS-12	0.718142	0.770826	0.771770	0.627353	-3990.732654	-3989.960884	-3990.105301	-1438.218
TS-13	0.718109	0.770941	0.771886	0.625561	-3990.722198	-3989.950312	-3990.096637	-1361.123
C-15	0.213232	0.226551	0.227495	0.173700	-658.074752	-657.847257	-657.901052	—
C-16	0.212867	0.226375	0.227319	0.172588	-658.074938	-657.847619	-657.902350	—
C-17	0.070198	0.073914	0.074858	0.043925	-229.992411	-229.917553	-229.948486	—
TS-14	0.180415	0.192718	0.193662	0.139781	-639.146017	-638.952355	-639.006236	-272.557
TS-15	0.180140	0.192390	0.193334	0.140308	-639.140180	-638.946846	-638.999872	-336.416
C-18	0.180629	0.192870	0.193814	0.142004	-639.181256	-638.987442	-639.039252	—

C-19	0.181005	0.193196	0.194140	0.142344	-639.166998	-638.972858	-639.024654	—
TS-16	0.678186	0.729187	0.730131	0.587893	-3971.302116	-3970.571985	-3970.714223	-309.649
TS-17	0.677737	0.729040	0.729984	0.586542	-3971.286984	-3970.557000	-3970.700442	-1165.662
C-20	0.172284	0.183880	0.184824	0.134582	-638.630092	-638.445268	-638.495510	—
C-21	0.172511	0.184049	0.184993	0.134807	-638.630715	-638.445722	-638.495908	—
C-22	0.066891	0.070965	0.071909	0.039651	-552.971110	-552.899201	-552.931459	—
TS-18	0.177137	0.189897	0.190841	0.135876	-962.125143	-961.934302	-961.989267	-274.439
TS-19	0.177017	0.189742	0.190686	0.135822	-962.122093	-961.931407	-961.986271	-293.261
C-23	0.178025	0.190635	0.191579	0.138778	-962.167273	-961.975694	-962.028495	—
C-24	0.177542	0.190377	0.191322	0.137913	-962.149559	-961.958237	-962.011646	—
TS-20	0.675217	0.726765	0.727710	0.584657	-4294.296401	-4293.568691	-4293.711744	-768.651
TS-21	0.674758	0.726363	0.727307	0.584144	-4294.275331	-4293.548024	-4293.691187	-1235.687
C-25	0.169277	0.181245	0.182189	0.130654	-961.611436	-961.429247	-961.480782	—
C-26	0.169085	0.181057	0.182001	0.130709	-961.608367	-961.426366	-961.477658	—
TS-4	0.507360	0.540242	0.541186	0.439261	-1455.162461	-1454.621275	-1454.723200	-963.547
TS-5	0.507779	0.540433	0.541377	0.440999	-1455.153606	-1454.612229	-1454.712607	-1056.197
TS-22	0.459612	0.489892	0.490836	0.396170	-1301.521651	-1301.030815	-1301.125481	-720.947
TS-23	0.459901	0.490029	0.490973	0.396665	-1301.510882	-1301.019909	-1301.114217	-976.234
TS-24	0.418983	0.447738	0.448682	0.356704	-1282.089431	-1281.640749	-1281.732727	-699.318
TS-25	0.420032	0.448384	0.449328	0.358172	-1282.078620	-1281.629292	-1281.720448	-933.954
TS-26	0.417154	0.446125	0.447069	0.354791	-1605.083443	-1604.636374	-1604.728652	-876.649
TS-27	0.417118	0.446017	0.446961	0.354836	-1605.066298	-1604.619337	-1604.711462	-995.807
TS-28	0.769959	0.823590	0.824535	0.681725	-2393.761697	-2392.937162	-2393.079972	-823.408

Cartesian coordinates of the structures

KOtBu

C	1.61010700	1.01764800	-1.04001700
C	1.07202700	0.00006500	-0.00009800
H	1.23720600	0.75376100	-2.03823200
H	1.23781900	2.02141000	-0.79701900
H	2.70796700	1.05905000	-1.08255000
C	1.61109200	0.39186400	1.40093900
C	1.60994700	-1.40984100	-0.36130400
H	1.23813600	-0.31922100	2.14954100
H	2.70904000	0.40639600	1.45700600
H	1.23997100	1.38906000	1.67139700
H	2.70776000	-1.46832900	-0.37355000
H	1.23451300	-2.14187700	0.36546100
H	1.23915100	-1.70074000	-1.35273600
O	-0.30080900	0.00007000	0.00000900
K	-2.55600700	0.00008000	0.00018400

[KOtBu]₂

K	-0.00039500	1.78010700	0.14098800
O	1.73934700	0.00038000	0.13409200
O	-1.73938200	-0.00052500	0.13447900
K	0.00035300	-1.78023100	0.14097600
C	3.10725800	0.00015200	-0.04675400
C	-3.10724800	-0.00012100	-0.04673500
C	3.83865800	0.00136600	1.31965000

H	4.93356700	0.00107400	1.22635600
H	3.54384000	0.88718500	1.89731500
H	3.54348200	-0.88322500	1.89899900
C	3.55269600	-1.25651500	-0.84377300
H	3.03047500	-1.28460600	-1.80937300
H	4.63329800	-1.29148500	-1.03821900
H	3.28812700	-2.16578600	-0.28377400
C	3.55277400	1.25527100	-0.84613700
H	4.63339100	1.28983800	-1.04057600
H	3.03057200	1.28157600	-1.81179300
H	3.28816100	2.16560700	-0.28789800
C	-3.83900700	-0.00354200	1.31946200
H	-3.54397800	0.88010200	1.90032200
H	-4.93389100	-0.00310800	1.22587600
H	-3.54434700	-0.89029800	1.89577000
C	-3.55258400	1.25777800	-0.84188300
H	-4.63314300	1.29298200	-1.03651800
H	-3.28821500	2.16617200	-0.28036500
H	-3.03016400	1.28742800	-1.80733200
C	-3.55242700	-1.25400100	-0.84824200
H	-3.28793100	-2.16521200	-0.29137100
H	-4.63298500	-1.28833400	-1.04305600
H	-3.02990900	-1.27873300	-1.81376300

[KOTBu]₃

O	0.00015600	1.99898400	-0.24404000
O	2.30339200	-0.91026700	-0.11571700
O	-2.30411900	-0.90944400	-0.11548200
K	-2.26639700	1.24327100	-1.24738100
K	2.26606000	1.24224500	-1.24814300
K	-0.00020800	-0.56204900	0.94732200
C	0.00059000	3.14890900	0.53473600
C	3.16018400	-1.98185400	0.04070200
C	-3.16059500	-1.98133200	0.04061100
C	-1.25165200	4.02460900	0.24927900
H	-2.16932900	3.48261300	0.52301200
H	-1.25793200	4.96449300	0.81609000
H	-1.29717900	4.27731700	-0.81940200
C	1.25368300	4.02348900	0.24957000
H	1.26073900	4.96329100	0.81650600
H	2.17081200	3.48060700	0.52337600
H	1.29960200	4.27631400	-0.81906900
C	0.00027300	2.79074600	2.04497300
H	0.89026300	2.19420700	2.28829200
H	0.00058600	3.67297100	2.69869900
H	-0.89027300	2.19496300	2.28810400
C	-4.63064600	-1.49411200	0.15035400
H	-4.91351900	-0.95694000	-0.76707100
H	-5.35112900	-2.31138700	0.29272500
H	-4.72764300	-0.79908600	0.99443600
C	-3.04955500	-2.94819200	-1.16615400
H	-2.01491100	-3.30061700	-1.26250500
H	-3.70717800	-3.82429700	-1.08088200
H	-3.30798200	-2.41724400	-2.09267400
C	-2.82034400	-2.77429200	1.33264900
H	-1.79361600	-3.16344500	1.27430400
H	-2.88873800	-2.10955600	2.20464100
H	-3.48765000	-3.62977200	1.50422400
C	3.04905500	-2.94938900	-1.16551200
H	3.70702300	-3.82521100	-1.08001000
H	2.01450200	-3.30223300	-1.26130200
H	3.30695200	-2.41884200	-2.09240900
C	4.63014600	-1.49420200	0.14976400

H	4.72717900	-0.79863700	0.99340000
H	5.35087800	-2.31120000	0.29245800
H	4.91266400	-0.95753000	-0.76806700
C	2.82050900	-2.77419000	1.33327200
H	2.88885700	-2.10893200	2.20486900
H	1.79390000	-3.16371700	1.27536900
H	3.48814700	-3.62934300	1.50519000

[KOTBu]₄

O	-1.35223000	-1.22398900	-1.39308300
O	1.33776900	-1.41923500	1.20966400
O	-1.29895000	1.23549700	1.43282500
O	1.31340800	1.40712700	-1.24975800
K	1.27675600	-1.21412600	-1.41362300
K	-1.29083300	-1.38866300	1.22775500
K	-1.31490700	1.39972200	-1.18877700
K	1.32898100	1.20247200	1.37432100
C	-2.17096600	-1.94544200	-2.24970100
C	2.14883000	-2.29018100	1.92258000
C	-2.08721500	1.96281600	2.31274900
C	2.10935200	2.27300200	-1.98552700
C	-1.89258000	-1.56766700	-3.72898400
H	-0.84297100	-1.77204500	-3.98192500
H	-2.52292000	-2.11815700	-4.44009400
H	-2.06704600	-0.49417300	-3.88575100
C	-3.66747600	-1.66064500	-1.95382900
H	-4.35011800	-2.21715100	-2.60988100
H	-3.90587600	-1.92758500	-0.91510700
H	-3.88178300	-0.58988600	-2.07707600
C	-1.92997000	-3.47011900	-2.08922200
H	-0.88052600	-3.71272900	-2.30610600
H	-2.13329200	-3.77922000	-1.05460000
H	-2.55996000	-4.07853500	-2.75185300
C	1.83813600	-3.76443600	1.55039700
H	1.99675500	-3.92581800	0.47513500
H	2.46150200	-4.48660800	2.09439300
H	0.78646900	-3.99726900	1.76767500
C	1.92916900	-2.12320100	3.44978300
H	2.55359700	-2.79699300	4.05164200
H	2.15595900	-1.09227600	3.75493600
H	0.87873600	-2.31959800	3.70516600
C	3.64714000	-2.02295400	1.61951400
H	3.90825500	-0.98855300	1.88195200
H	4.32386700	-2.69102000	2.16890000
H	3.84633300	-2.15169300	0.54648000
C	1.83962800	2.11308400	-3.50544100
H	0.78355000	2.32039100	-3.72671300
H	2.45104900	2.78284100	-4.12490100
H	2.04657300	1.08102000	-3.82059900
C	1.82430000	3.74880800	-1.59920300
H	2.01885500	3.90533800	-0.52912000
H	2.43652100	4.46703100	-2.16079400
H	0.76838600	3.99187500	-1.78187900
C	3.61401200	1.99110000	-1.73114300
H	3.84836800	2.11430600	-0.66458900
H	3.85711100	0.95527600	-2.00502600
H	4.27906900	2.65484500	-2.29968500
C	-1.83877100	3.48563800	2.14612900
H	-2.44463500	4.09861700	2.82681300
H	-0.78163800	3.71971100	2.33291200
H	-2.06920200	3.79703800	1.11789400
C	-3.59377600	1.69013700	2.05955700
H	-3.81305500	0.62103900	2.18837700

H	-4.25291300	2.25161800	2.73510900
H	-3.85963200	1.95971200	1.02820200
C	-1.76980400	1.58183100	3.78332400
H	-1.94855300	0.50970400	3.94460500
H	-0.71175700	1.77741800	4.00622400
H	-2.37504500	2.13699300	4.51238200

NaOtBu

C	1.14721600	1.45528400	-0.01297000
C	0.61947700	-0.00001700	-0.00006800
H	0.77577000	1.97449500	-0.90533400
H	0.77319000	1.99106000	0.86845300
H	2.24439000	1.51313900	-0.01193300
C	1.14518000	-0.71563600	1.26792800
C	1.14957800	-0.73951700	-1.25250600
H	0.77266300	-1.74741100	1.28993500
H	2.24227800	-0.74372100	1.32061800
H	0.77029800	-0.20292800	2.16258500
H	2.24687000	-0.76732400	-1.30104300
H	0.77827400	-1.77197300	-1.25577900
H	0.77708800	-0.24467100	-2.15813500
O	-0.75940500	-0.00017100	-0.00229800
Na	-2.69766200	0.00000100	-0.00048000

[NaOtBu]₂

O	1.59627900	0.00013400	0.08503200
O	-1.59628600	-0.00034600	0.08495900
C	2.98355300	0.00005400	-0.01459600
C	-2.98355100	-0.00003900	-0.01477900
C	3.61681700	0.00079700	1.39514900
H	4.71446500	0.00070700	1.36790200
H	3.28736500	0.88677800	1.95262300
H	3.28723300	-0.88451200	1.95360800
C	3.45898900	-1.25666500	-0.78252900
H	2.99659300	-1.27947000	-1.77750500
H	4.54867600	-1.29587800	-0.90919400
H	3.15304900	-2.16311700	-0.24069700
C	3.45902700	1.25591000	-0.78390500
H	4.54871200	1.29493100	-0.91063900
H	2.99658300	1.27766000	-1.77887900
H	3.15313100	2.16296000	-0.24305700
C	-3.61693000	-0.00294700	1.39491300
H	-3.28720200	0.88138500	1.95482700
H	-4.71457400	-0.00259900	1.36757600
H	-3.28771200	-0.88990200	1.95098100
C	-3.45886800	1.25792900	-0.78075300
H	-4.54854400	1.29741900	-0.90740900
H	-3.15289600	2.16349800	-0.23746200
H	-2.99644100	1.28227300	-1.77568200
C	-3.45902500	-1.25464100	-0.78611700
H	-3.15324000	-2.16257000	-0.24668200
H	-4.54870000	-1.29338800	-0.91302400
H	-2.99645900	-1.27485100	-1.78106400
Na	-0.00018500	1.41459500	0.09327900
Na	0.00017900	-1.41477800	0.09304300

[NaOtBu]₃

O	0.02156900	1.86375700	-0.39069100
O	2.05954600	-0.76137900	-0.03349500
O	-2.09149100	-0.71144400	-0.08200900
C	0.03590500	3.11875700	0.23915600
C	2.97151500	-1.80996700	0.04157400
C	-3.01974500	-1.74054600	0.04611900

C	-1.04531000	4.04107400	-0.37573100
H	-2.05156300	3.63181000	-0.19217500
H	-1.03737000	5.05202200	0.05015200
H	-0.89563300	4.12639500	-1.45988000
C	1.41471500	3.80110000	0.05158500
H	1.46289400	4.79884600	0.50409400
H	2.20606600	3.20065700	0.52598000
H	1.64065600	3.91346400	-1.01910500
C	-0.23659300	2.96186000	1.75184000
H	0.53415300	2.32851400	2.20936100
H	-0.24355800	3.92266400	2.28217300
H	-1.20873600	2.47811200	1.91185400
C	-4.45745700	-1.17432300	-0.04443800
H	-4.60420900	-0.68302300	-1.01764000
H	-5.23041600	-1.94725300	0.05793500
H	-4.61354700	-0.42661500	0.74372800
C	-2.81748400	-2.78204500	-1.07824200
H	-1.80155200	-3.19279800	-1.02906100
H	-3.52943000	-3.61591300	-1.01795600
H	-2.93584700	-2.30130500	-2.05818900
C	-2.85094100	-2.43918700	1.41680700
H	-1.84353300	-2.87034500	1.49584100
H	-2.97326400	-1.70674600	2.22462900
H	-3.57493000	-3.24949400	1.57350700
C	2.42951400	-3.04220500	-0.71887700
H	3.12049200	-3.89532100	-0.69424700
H	1.47584000	-3.36334300	-0.28078800
H	2.24278600	-2.77983300	-1.76773400
C	4.32071700	-1.38890000	-0.59162100
H	4.72336500	-0.51347700	-0.06350700
H	5.07883500	-2.18210700	-0.55626600
H	4.16883900	-1.11918900	-1.64689800
C	3.21852100	-2.19140400	1.52010600
H	3.58933600	-1.31926100	2.07249200
H	2.27662000	-2.51010100	1.98603300
H	3.94468700	-3.00726000	1.63312100
Na	-1.94968600	1.14968300	-1.02837200
Na	-0.01849800	-0.45107900	0.53813600
Na	2.00290100	1.11759100	-0.96136000

[NaOtBu]₄

O	1.11330300	-1.15663000	-1.26273000
O	-1.73097700	-0.98967600	0.47161100
O	-0.46237700	1.76602200	-0.91121300
O	1.05880200	0.36050300	1.70742100
C	1.87642300	-1.94427100	-2.12795000
C	-2.90698700	-1.65775500	0.82109000
C	-0.78216600	2.97013400	-1.54306300
C	1.81569300	0.63437400	2.84914300
C	2.14289800	-3.32995400	-1.49377000
H	1.18966800	-3.83418700	-1.28443500
H	2.73773900	-3.98893600	-2.13939800
H	2.68696400	-3.20967700	-0.54656000
C	3.23398100	-1.25930300	-2.41484200
H	3.87453700	-1.84283800	-3.08843500
H	3.06722300	-0.27723400	-2.87909800
H	3.78232900	-1.10926700	-1.47477800
C	1.12718600	-2.14510900	-3.46656200
H	0.16755800	-2.64936500	-3.28615100
H	0.92445300	-1.17011600	-3.93046900
H	1.69234100	-2.74953200	-4.18775400
C	-2.57226800	-3.02471200	1.46395800
H	-1.96364200	-2.87389400	2.36647000

H	-3.46561500	-3.59280200	1.75381300
H	-1.99796600	-3.63922200	0.75718100
C	-3.77782400	-1.89724500	-0.43493400
H	-4.71732200	-2.41897100	-0.21156700
H	-4.02977200	-0.93598500	-0.90338200
H	-3.22284400	-2.50282200	-1.16477100
C	-3.71740600	-0.81611300	1.83550500
H	-3.97596400	0.15594000	1.39292300
H	-4.65179000	-1.30160300	2.14531500
H	-3.11620000	-0.63801600	2.73771600
C	3.08752700	1.42943900	2.46759400
H	2.80627200	2.37405000	1.98185400
H	3.71672100	1.67233000	3.33340600
H	3.69701700	0.84474200	1.76440100
C	0.98680700	1.47307800	3.85050400
H	0.08068000	0.92285000	4.13848400
H	1.53980900	1.71435600	4.76737700
H	0.68297800	2.41990800	3.38282600
C	2.24193600	-0.68466100	3.53605600
H	1.35188000	-1.26017600	3.82549200
H	2.83610900	-1.29299700	2.84036500
H	2.84465100	-0.52181800	4.43879600
C	0.50507800	3.77713600	-1.83560600
H	0.30563200	4.73944300	-2.32429300
H	1.03930300	3.98025200	-0.89738200
H	1.16825400	3.19835700	-2.49355700
C	-1.51156000	2.69479000	-2.87943200
H	-2.43733600	2.13325700	-2.69153700
H	-1.78063200	3.61319300	-3.41691900
H	-0.86942800	2.09474300	-3.53858100
C	-1.70679600	3.81845900	-0.63775400
H	-2.62885100	3.26213700	-0.42029500
H	-1.20161800	4.03705700	0.31335100
H	-1.99107600	4.77570700	-1.09321100
Na	0.40921400	-1.60661800	0.82665400
Na	-1.01458200	1.03498300	1.14947700
Na	1.55338600	0.89104100	-0.42966100
Na	-0.96867300	-0.33761800	-1.54170100
[KOTBu]₃K⁺			
O	2.05158400	-0.56506200	-0.19895100
O	-1.51439300	-1.49425000	-0.19894200
O	-0.53689700	2.05807700	-0.19801700
K	1.82502400	1.80047300	-1.23403600
K	0.64746800	-2.48255100	-1.23409100
K	-2.47290800	0.68077600	-1.23475200
K	-0.00029000	-0.00121300	1.42548400
C	3.31049500	-0.90980400	0.30659200
C	-2.44401100	-2.41046400	0.30675100
C	-0.86609400	3.32143500	0.30684000
C	4.39740100	0.09028000	-0.16636300
H	4.18706000	1.10046100	0.21701700
H	5.40184400	-0.17440900	0.18385800
H	4.43097800	0.12543700	-1.26464500
C	3.73646100	-2.32410200	-0.16650100
H	4.73563700	-2.60775900	0.18399700
H	3.04082300	-3.08647700	0.21623900
H	3.74798200	-2.37117800	-1.26480600
C	3.29413000	-0.90589600	1.85616000
H	2.55432200	-1.62839300	2.22994500
H	4.26225400	-1.17189900	2.29733900
H	3.02680400	0.09259700	2.23107100
C	0.14785800	4.39542900	-0.16606000

H	0.18351100	4.42866100	-1.26433600
H	-0.10399100	5.40313200	0.18409600
H	1.15510600	4.17177200	0.21738600
C	-2.27489600	3.76434600	-0.16704700
H	-3.04560800	3.07819700	0.21610700
H	-2.54712700	4.76720400	0.18207600
H	-2.32149100	3.77542400	-1.26539800
C	-0.86279900	3.30573800	1.85637900
H	-1.59539300	2.57605700	2.23037700
H	0.13180800	3.02463800	2.23161900
H	-1.11550300	4.27777400	2.29679500
C	-3.88253600	-2.06284600	-0.15696700
H	-4.63010100	-2.78354000	0.19437100
H	-4.18753000	-1.07916600	0.23152200
H	-3.93502200	-2.04479100	-1.25499900
C	-2.13038100	-3.85076700	-0.17514900
H	-1.14997500	-4.17998000	0.20172900
H	-2.86334300	-4.58679000	0.17506500
H	-2.12215900	-3.89193600	-1.27366500
C	-2.42421700	-2.40660000	1.85635800
H	-1.42458400	-2.67910600	2.22453600
H	-2.67538100	-1.40621200	2.23735800
H	-3.13832400	-3.11254500	2.29715900
tBuO⁻			
C	0.76990700	-1.24423200	-0.43646700
C	-0.00013200	0.00003900	0.15967000
H	1.80129600	-1.23055200	-0.05612200
H	0.29633500	-2.16128700	-0.05785000
H	0.80755900	-1.30304500	-1.54066300
C	-1.46233400	-0.04419800	-0.43746700
C	0.69327500	1.28854000	-0.43640400
H	-2.02015500	0.82358000	-0.05747100
H	-1.53137600	-0.04520400	-1.54167000
H	-1.96645600	-0.94501600	-0.05922000
H	0.72747800	1.34879700	-1.54055500
H	0.16518700	2.17550300	-0.05815900
H	1.72349000	1.33736900	-0.05572100
O	-0.00095700	-0.00012900	1.48392900
O₂			
O	0.00000000	0.00000000	0.60729600
O	0.00000000	0.00000000	-0.60729600
HSiMe₃			
C	-1.65115200	-0.70715200	-0.22213800
H	-1.70164300	-0.72877000	-1.31767000
H	-1.79886000	-1.73251900	0.13686300
H	-2.49495200	-0.10599200	0.13664300
C	0.21304900	1.78332800	-0.22197400
H	-0.60064800	2.42400000	0.13790700
H	1.15591300	2.21328500	0.13607500
H	0.21849900	1.83815500	-1.31758600
C	1.43828700	-1.07596800	-0.22208500
H	2.40001400	-0.68949200	0.13542000
H	1.34133200	-2.10693900	0.13817300
H	1.48118200	-1.11009300	-1.31764100
Si	-0.00013800	-0.00018300	0.37553700
H	-0.00001200	-0.00031900	1.87147700
Me₃Si•			
C	-1.49707800	-1.00822500	0.17717800
H	-1.53730000	-1.03547100	1.27530500

H	-2.43733300	-0.57387800	-0.18009200
H	-1.44975600	-2.04264900	-0.18063800
C	1.62207500	-0.79159600	0.17728500
H	1.71822300	-1.82261600	-0.18070000
H	2.49329800	-0.23134900	-0.17964300
H	1.66499200	-0.81318200	1.27540400
C	-0.12521400	1.80036000	0.17698200
H	0.72164900	2.39781100	-0.17838200
H	-1.04408300	2.27602000	-0.18319200
H	-0.13146500	1.84922500	1.27520600
Si	0.00022000	-0.00051000	-0.42371000

H₂

H	0.00000000	0.00000000	0.37139400
H	0.00000000	0.00000000	-0.37139400

Me•

C	0.00000000	0.00000000	0.00015500
H	0.00000000	1.08279800	-0.00031000
H	-0.93773100	-0.54139900	-0.00031000
H	0.93773100	-0.54139900	-0.00031000

tBuO•

C	1.28444000	-0.78208500	-0.31507600
C	0.00040800	-0.02651100	0.08147400
H	2.16791400	-0.20844400	-0.01830000
H	1.32075100	-1.75298600	0.19083000
H	1.32290000	-0.95893000	-1.39608100
C	-1.27108600	-0.80336200	-0.31547500
C	-0.01160200	1.38844700	-0.57944400
H	-2.16376300	-0.24501700	-0.01726300
H	-1.30694300	-0.97930400	-1.39670400
H	-1.29060700	-1.77542800	0.18915300
H	-0.00952400	1.26142700	-1.66749800
H	-0.90726600	1.94171900	-0.28474700
H	0.87381300	1.95737200	-0.28347000
O	-0.00253000	0.26258200	1.43190100

tBuOH

C	1.49029100	-0.03159600	-0.35612300
C	0.00542200	-0.00042200	0.01380400
H	2.00202100	0.84324500	0.05811700
H	1.96432400	-0.92932300	0.05413200
H	1.62279900	-0.03227900	-1.44334000
C	-0.71772600	-1.24971300	-0.51177000
C	-0.66220400	1.28083700	-0.50917000
H	-1.77526300	-1.24080000	-0.21558600
H	-0.68154600	-1.30568500	-1.60601700
H	-0.25727900	-2.15453300	-0.10156900
H	-0.62395000	1.33693200	-1.60339300
H	-1.71884100	1.31844800	-0.21227200
H	-0.16130100	2.16324100	-0.09761100
O	-0.01498900	-0.00165100	1.45245600
H	-0.94575600	0.01932100	1.72744200

tBuOSiMe₃

C	-1.53411400	-1.23720200	-1.35238600
H	-2.59102300	-1.23736700	-1.64901100
H	-0.94667900	-0.99675900	-2.24657300
H	-1.27718400	-2.25866200	-1.04848800
C	-2.31725500	-0.48686300	1.53679500
H	-2.06466900	-1.49251500	1.89193600
H	-2.16594600	0.20684700	2.37180400

H	-3.38473400	-0.47823700	1.28369500
C	-1.75796900	1.72368900	-0.53265700
H	-1.58137700	2.47348600	0.24773200
H	-1.20820700	2.03791000	-1.42690700
H	-2.82757300	1.74880900	-0.77830300
Si	-1.25814100	-0.00315800	0.05651400
C	1.99831700	-1.41884400	-0.37810500
C	1.61900600	0.00048500	0.07176700
H	1.90998800	-2.11544200	0.46213300
H	1.34135400	-1.76589300	-1.18235000
H	3.03071900	-1.45003700	-0.74568900
C	1.68847800	0.98094200	-1.10862100
C	2.54983700	0.46578500	1.19983800
H	1.38888700	1.98590600	-0.79350800
H	2.70933600	1.03649600	-1.50346100
H	1.03245900	0.66474500	-1.92773700
H	3.59362700	0.48878300	0.86633100
H	2.26852800	1.46969900	1.53483400
H	2.47200200	-0.21288500	2.05537100
O	0.30458100	-0.02857800	0.64715000
TS1			
C	-2.14636800	-1.41577200	-1.15357100
H	-3.22466700	-1.47711600	-1.35135600
H	-1.64000700	-1.28333700	-2.11644200
H	-1.82917400	-2.37852800	-0.73730500
C	-2.61552300	-0.26914600	1.70646900
H	-2.31800600	-1.22614900	2.14927300
H	-2.35401000	0.52230100	2.41755100
H	-3.70772500	-0.27475200	1.59554300
C	-2.23281000	1.67780700	-0.70170800
H	-1.97024200	2.49659800	-0.02251200
H	-1.72152400	1.85604400	-1.65455300
H	-3.31339200	1.73222300	-0.88855300
Si	-1.76254300	0.00178500	0.04194100
H	-0.17719900	0.00403800	0.37408200
C	3.37885900	-0.00601000	0.88779900
C	2.08839900	0.00073400	0.03482300
H	3.41089900	0.87516300	1.53591300
H	3.41488200	-0.90044100	1.51728300
H	4.26064400	0.00283300	0.23639000
C	2.03621200	-1.25987200	-0.84640900
C	2.03476000	1.27819100	-0.82186600
H	1.12007400	-1.27049600	-1.44851900
H	2.89099100	-1.30702200	-1.53199300
H	2.04129800	-2.15765300	-0.21954600
H	2.89098200	1.34069900	-1.50436700
H	1.12002600	1.29785700	-1.42603600
H	2.03580300	2.16356900	-0.17772100
O	1.06059600	-0.00955200	1.00405800
KOO•			
O	0.67492300	-1.27141100	0.00000000
O	-0.67492300	-1.27056800	0.00000000
K	0.00000000	1.07030700	0.00000000
[KOTBu] KOO•			
K	1.08630200	-1.84918300	0.03516300
O	-0.59874800	0.00015900	0.11880200
O	2.81050400	-0.00008000	0.62476000
K	1.08652900	1.84918400	0.03514300
C	-1.97321600	0.00003900	0.00097300
C	-2.64260900	-0.00003800	1.39900000

H	-3.74058000	0.00012500	1.35488900
H	-2.32145100	-0.88506900	1.96359500
H	-2.32119800	0.88473900	1.96385100
C	-2.45598300	1.25567700	-0.77661700
H	-1.97798900	1.28339000	-1.76482400
H	-3.54427200	1.29024000	-0.92209100
H	-2.16818300	2.16592100	-0.22929800
C	-2.45581400	-1.25561100	-0.77671900
H	-3.54405500	-1.29010000	-0.92256200
H	-1.97748300	-1.28346600	-1.76476100
H	-2.16829600	-2.16584400	-0.22922800
O	2.74392500	-0.00012100	-0.72671000

[KOtBu]₃KOO• (C-2)

O	0.02988400	-0.11123300	2.75134900
O	2.02055500	-0.82028400	-0.18396600
O	-0.33038300	2.05201500	-0.32802400
O	-1.66346100	-1.40888300	-0.17022400
K	0.35285300	-2.18278800	1.28871600
K	1.70099800	1.40359700	1.24764900
K	-2.04373800	0.80469500	1.26266700
K	0.01440400	-0.10984400	-1.73244700
C	3.26257100	-1.27660700	-0.59079000
C	-0.53791300	3.32923700	-0.81978300
C	-2.70717800	-2.21869700	-0.58387700
C	3.54262300	-2.69690100	-0.02734900
H	2.77701100	-3.39930400	-0.38739700
H	4.52250200	-3.09623800	-0.32113600
H	3.50738800	-2.67623700	1.07134000
C	4.38985400	-0.33235700	-0.09094200
H	5.39471700	-0.65811500	-0.39074400
H	4.23487500	0.67912700	-0.49279800
H	4.37162500	-0.27792800	1.00698100
C	3.34478200	-1.34798900	-2.13946700
H	3.17315100	-0.35048900	-2.56793900
H	4.31496600	-1.70741600	-2.50780300
H	2.56942900	-2.02665200	-2.52221900
C	-2.52766900	-3.66728600	-0.05327800
H	-2.49258000	-3.66090900	1.04561700
H	-3.33695400	-4.34492000	-0.35621300
H	-1.58382600	-4.08802800	-0.42901800
C	-4.06642200	-1.68063700	-0.05897500
H	-4.23828800	-0.66443800	-0.44187300
H	-4.92385400	-2.29714500	-0.36002700
H	-4.05299300	-1.64226300	1.03961900
C	-2.78007900	-2.27862100	-2.13364400
H	-2.92771100	-1.26746900	-2.53850000
H	-1.83870700	-2.67887400	-2.53615800
H	-3.59759200	-2.91005300	-2.50663800
C	-0.54944900	3.32789400	-2.37275600
H	-0.71465600	4.32284600	-2.80762400
H	0.41174800	2.95293400	-2.75247300
H	-1.34822900	2.66712800	-2.73872700
C	-1.89743700	3.89900200	-0.32986600
H	-1.91417900	3.93445800	0.76842500
H	-2.10017900	4.91324200	-0.69898200
H	-2.71804900	3.25148300	-0.67109800
C	0.58382200	4.29439400	-0.34777900
H	0.60444900	4.33474000	0.75033300
H	1.56004000	3.93338100	-0.70240000
H	0.45609400	5.32103600	-0.71618400
O	-0.17172700	1.15463300	3.15455800

NaOO•

O	1.04416800	0.20075100	0.00000000
O	0.00000000	1.06326600	0.00000000
Na	-0.75939500	-0.91928500	0.00000000

[NaOtBu]NaOO•

O	0.34168700	-0.04804000	0.00146000
O	-2.97506000	0.01925700	-0.68027200
C	1.73345000	-0.00684500	0.00004400
C	2.28180200	-0.72616400	-1.25311000
H	3.37765500	-0.70028700	-1.31324800
H	1.96881600	-1.77905300	-1.24711600
H	1.87429000	-0.25987500	-2.15819400
C	2.21730100	1.46341600	-0.01808500
H	1.83841300	1.99163300	0.86793000
H	3.31101000	1.55473900	-0.02037100
H	1.83614100	1.97030300	-0.91542400
C	2.28354200	-0.69594400	1.26924300
H	3.37948100	-0.66845800	1.32723600
H	1.87722400	-0.20818600	2.16348900
H	1.97054800	-1.74860700	1.28908800
O	-2.97643700	0.01926900	0.67886000
Na	-1.23087400	1.37739400	0.00077600
Na	-1.28291400	-1.40311000	0.00083100

[NaOtBu]3NaOO• (C-3)

O	0.09058800	0.67535300	2.92791900
O	-0.91597200	1.66045600	-0.12729800
O	-0.91801000	-1.65959800	-0.12683000
O	1.92934200	-0.00128300	-0.13775700
C	-1.69194100	2.75776900	-0.51473100
C	-1.69519100	-2.75595900	-0.51453200
C	3.26107500	-0.00190900	-0.56984500
C	-1.00053400	4.07525000	-0.09153500
H	-0.00947000	4.14498100	-0.56122200
H	-1.57002500	4.96841300	-0.37854400
H	-0.87158100	4.09757800	0.99945400
C	-3.08415100	2.68890500	0.15665500
H	-3.73180400	3.53199900	-0.11557000
H	-3.59814100	1.76408500	-0.14021600
H	-2.97355100	2.69211400	1.24985900
C	-1.87756400	2.76111100	-2.04985000
H	-2.37500100	1.83477800	-2.36797400
H	-2.48070900	3.60604300	-2.40599500
H	-0.89794900	2.81520100	-2.54455600
C	3.99290000	1.25494900	-0.04219500
H	3.96540600	1.27219600	1.05621300
H	5.04531800	1.29829700	-0.34967100
H	3.50078600	2.16254800	-0.42040800
C	3.99175700	-1.25937400	-0.04207700
H	3.49877300	-2.16655300	-0.42015200
H	5.04412000	-1.30373100	-0.34959500
H	3.96428800	-1.27646600	1.05633300
C	3.31732400	-0.00200400	-2.11478100
H	2.80734900	-0.89251700	-2.50685400
H	2.80812600	0.88891500	-2.50693900
H	4.34297700	-0.00247100	-2.50508000
C	-1.88340200	-2.75699600	-2.04934200
H	-2.48782800	-3.60093300	-2.40566600
H	-2.38058500	-1.82979800	-2.36532500
H	-0.90466600	-2.81122100	-2.54579000
C	-1.00373100	-4.07439000	-0.09440600
H	-0.87317900	-4.09847700	0.99636000

H	-1.57403700	-4.96686400	-0.38193600
H	-0.01339100	-4.14377300	-0.56564500
C	-3.08623400	-2.68734900	0.15929400
H	-2.97378100	-2.69182700	1.25229300
H	-3.60040600	-1.76200000	-0.13563700
H	-3.73466400	-3.52987600	-0.11283500
O	0.08952300	-0.67460900	2.92798300
Na	-1.55514400	0.00099900	1.27724300
Na	0.98195300	-1.65375800	1.03775600
Na	0.98399000	1.65275000	1.03726900
Na	-0.00825300	-0.00028300	-1.31890000

[KOtBu]HSiMe₃

C	-1.90583800	0.41794000	1.54268800
H	-0.81654300	0.27981200	1.46868100
H	-2.15111600	1.48750700	1.63399500
H	-2.25265500	-0.06226900	2.46484900
C	-2.39966200	-2.22698700	-0.00172200
H	-2.83964800	-2.70198800	0.88296500
H	-2.83945200	-2.69965500	-0.88775400
H	-1.32477200	-2.44172100	-0.00205100
C	-1.90882300	0.42192800	-1.54112600
H	-2.25881400	-0.05478400	-2.46389300
H	-2.15341600	1.49203800	-1.62811500
H	-0.81943600	0.28259100	-1.47086600
Si	-2.68538600	-0.36189000	0.00058400
H	-4.15836700	-0.08549000	0.00213300
O	1.13393500	0.30748900	-0.00293900
C	2.15257400	-0.62244700	-0.00023700
C	3.53301800	0.08313100	-0.08140100
H	4.38128600	-0.61581100	-0.08703500
H	3.58417600	0.68720000	-0.99750900
H	3.65415500	0.75690300	0.77795900
C	2.11156400	-1.46610300	1.29958200
H	2.20276000	-0.80540300	2.17149000
H	1.14853800	-1.98622500	1.37419100
H	2.91242100	-2.21701400	1.35154000
C	2.01995900	-1.57452500	-1.21627000
H	1.05565700	-2.09615700	-1.17553300
H	2.04535500	-0.99204100	-2.14622900
H	2.81725300	-2.32963200	-1.26065600
K	0.24841000	2.44795100	-0.00010000

TS29

C	1.92503200	-0.92101300	-0.97696900
H	2.81852600	-1.08402200	-0.35805200
H	1.57499300	-1.89906500	-1.32297800
H	2.22623500	-0.33400400	-1.85089100
C	1.09478000	1.72088700	0.50075100
H	1.27789300	2.32851400	-0.39229200
H	0.30662400	2.20460600	1.08521800
H	2.01709800	1.72052500	1.09647200
C	-0.20157500	-1.06261300	1.37280800
H	-0.04091700	-0.64359500	2.37220300
H	-1.29130300	-1.03637600	1.17619600
H	0.13555600	-2.10359100	1.36242300
Si	0.60092900	-0.03309900	0.04461900
H	-0.66502200	0.02705000	-1.14457700
O	-1.65236000	0.58648200	-0.74741000
O	-2.55790400	-0.22900900	-0.25608000

HOO•

O	0.05589000	-0.61174300	0.00000000
---	------------	-------------	------------

O	0.05589000	0.72018700	0.00000000
H	-0.89424400	-0.86754600	0.00000000
[tBuOSiHMe₃]⁻			
C	-1.29845800	1.70118700	-0.98968200
H	-2.12059400	2.36318200	-0.68128800
H	-0.35128400	2.22230400	-0.80311300
H	-1.41034200	1.56868100	-2.07673500
C	-1.29880500	-1.70152100	-0.98909400
H	-1.40858400	-1.56882600	-2.07635100
H	-0.35243000	-2.22353100	-0.80093200
H	-2.12215200	-2.36271100	-0.68224700
C	-2.16147300	0.00037100	1.73191600
H	-2.80117500	-0.87967200	1.89304900
H	-1.36320100	0.00137400	2.48065000
H	-2.80286100	0.87930600	1.89231500
Si	-1.52596800	0.00002200	-0.08760900
C	1.63870500	-0.00111900	-1.43250000
C	1.53036100	-0.00001300	0.11613800
H	1.15631400	-0.88697800	-1.85710800
H	1.15517300	0.88347000	-1.85845200
H	2.69110300	-0.00069100	-1.75349500
C	2.26446600	1.25806400	0.65161500
C	2.26521000	-1.25687800	0.65340600
H	2.20482200	1.27247500	1.74650500
H	3.32508100	1.29415600	0.35751900
H	1.77134300	2.16382700	0.27966300
H	3.32578000	-1.29294300	0.35914700
H	2.20579300	-1.26966100	1.74833000
H	1.77236300	-2.16339100	0.28292700
O	0.23727500	-0.00017100	0.61796400
H	-3.04983800	0.00014800	-0.61836500
[tBuOSiMe₃]^{-•}			
C	2.81747600	0.08020000	1.33350000
H	3.78867100	0.09828200	0.79919400
H	2.77108000	0.98435600	1.95984800
H	2.83677300	-0.78096600	2.01908400
C	1.82129900	-1.55331400	-0.92294300
H	1.73260000	-2.48303900	-0.34176700
H	1.22232600	-1.68062600	-1.83291200
H	2.87894000	-1.45692000	-1.21440900
C	1.67813700	1.51550200	-0.99944600
H	1.10680100	1.50832500	-1.93615400
H	1.44905300	2.46190800	-0.48749500
H	2.75062900	1.53782000	-1.24963600
Si	1.21951700	-0.01896900	0.09667100
C	-1.92333100	-1.10233900	1.16259500
C	-1.74114200	-0.01080600	0.07912600
H	-1.83966000	-2.09535500	0.70397400
H	-1.12619300	-1.00937700	1.90855600
H	-2.90052700	-1.02951600	1.66570100
C	-1.86593400	1.38404900	0.73995400
C	-2.85934000	-0.16379900	-0.97636900
H	-1.73740400	2.16682200	-0.01761400
H	-2.84376000	1.52568700	1.22689600
H	-1.07448300	1.50573700	1.48803200
H	-3.86449300	-0.07039200	-0.53679100
H	-2.74359800	0.60239300	-1.75248100
H	-2.77806800	-1.14461400	-1.46011700
O	-0.53311500	-0.15898900	-0.59922700
[tBuOSiMe₃][•]K⁺			

C	2.38384600	-0.65420300	1.36085800
H	3.08984700	-1.49460900	1.38370300
H	2.97385500	0.25827200	1.21953000
H	1.90861100	-0.59892800	2.34700500
C	0.20774900	-2.56153100	0.34965600
H	-0.35185500	-2.52437800	1.29289800
H	-0.49039100	-2.83794400	-0.45136700
H	0.93025200	-3.38377500	0.43546700
C	1.98115200	-1.09868900	-1.67618400
H	1.25498500	-1.20645300	-2.49082600
H	2.62134600	-0.24138500	-1.90899000
H	2.61560200	-1.99447700	-1.68242300
Si	1.11189300	-0.94523700	-0.00638900
C	0.11901100	2.13185300	1.45743300
C	-0.01485000	1.67837700	-0.00318700
H	-0.70659300	1.73093200	2.05541900
H	1.06018500	1.78716700	1.89641500
H	0.09273800	3.22549300	1.52674700
C	1.16729300	2.18153400	-0.84433200
C	-1.32449300	2.20670300	-0.60129700
H	1.08022400	1.84041100	-1.88090400
H	1.18675700	3.27690500	-0.84696100
H	2.12659700	1.83802400	-0.44276900
H	-1.31461400	3.30138600	-0.64960000
H	-1.47264000	1.81875800	-1.61528500
H	-2.18500100	1.91542600	0.01372100
O	-0.10826200	0.22828800	-0.03611700
K	-2.95992400	-0.97937200	-0.00426700

N-Me-Indole (1)

C	-0.65997000	-1.47306500	0.00003600
C	0.15148500	-0.33261200	-0.00000400
C	-0.38888200	0.98515800	-0.00002600
C	-1.78526900	1.14347500	-0.00002200
C	-2.59400200	0.01418700	-0.00001000
C	-2.03700600	-1.28114200	0.00002000
H	-0.23536700	-2.47317700	0.00006200
H	-2.22476500	2.13780600	-0.00000900
H	-3.67479400	0.12696900	-0.00000200
H	-2.69562200	-2.14541600	0.00003700
C	0.72629300	1.88868700	0.00005800
C	1.86038200	1.12059200	-0.00006600
H	2.90090000	1.41719200	-0.00009100
N	1.52953700	-0.22374500	-0.00005000
H	0.69119300	2.96943400	0.00003900
C	2.45994500	-1.33308700	0.00004000
H	2.32730100	-1.95880400	0.89078500
H	2.32691100	-1.95921700	-0.89035100
H	3.47962300	-0.94173300	-0.00028000

TS-2

C	-2.59032400	1.09620600	0.58236100
C	-1.56148600	0.61479800	-0.23249000
C	-1.50372500	-0.75092100	-0.65013000
C	-2.53482200	-1.62607700	-0.25564800
C	-3.56644400	-1.14226600	0.53909900
C	-3.59232800	0.20283800	0.95752900
H	-2.61673500	2.13059200	0.91310800
H	-2.51825900	-2.66710600	-0.56827300
H	-4.36495500	-1.81086200	0.84938500
H	-4.40725500	0.55140700	1.58608200
C	-0.32371400	-0.89434200	-1.43349000
C	0.34856000	0.33519100	-1.40958900

H	1.07105800	0.69185200	-2.13267200
N	-0.47525700	1.27554400	-0.77581600
H	0.01733100	-1.78538800	-1.94275300
Si	2.33151200	-0.22844300	0.27902400
C	1.46235600	-1.02968200	1.76605300
H	0.67442400	-1.71554900	1.43870400
H	2.17668200	-1.59867900	2.37728900
H	0.99697100	-0.27627000	2.41171700
C	3.62509400	1.03434800	0.90259000
H	4.40133200	0.53507500	1.50072000
H	4.12622200	1.54318400	0.07087400
H	3.16375600	1.80194700	1.53448500
C	3.23580400	-1.55825700	-0.74111300
H	3.74581400	-1.12380700	-1.60931400
H	3.99693000	-2.06540400	-0.13236700
H	2.54223900	-2.32306800	-1.10771800
C	-0.07021500	2.62364900	-0.44907500
H	0.43863400	2.67716300	0.52433800
H	0.61420700	2.99184900	-1.21807200
H	-0.94530700	3.27956000	-0.42773700

TS-3

C	-2.81248500	-0.08347300	0.64832900
C	-1.70313500	0.37539800	-0.06930500
C	-0.87271800	-0.50187100	-0.81466500
C	-1.18858500	-1.86328200	-0.85880400
C	-2.30439000	-2.32640300	-0.16263700
C	-3.10238100	-1.44503200	0.58682200
H	-3.43213300	0.59211200	1.23110500
H	-0.56616900	-2.55264100	-1.42393800
H	-2.55876500	-3.38222200	-0.19426400
H	-3.96159100	-1.83033700	1.12930500
C	0.22111900	0.29978100	-1.36513800
C	-0.10740900	1.62840000	-1.05182000
H	0.39660300	2.54635600	-1.31917300
N	-1.21716500	1.66502300	-0.21928800
C	-1.73728900	2.83687600	0.44914600
H	-2.82606400	2.88791000	0.33733500
H	-1.49575800	2.83725600	1.52070600
H	-1.30325200	3.73001100	-0.00663100
H	0.77378300	0.03195000	-2.25682400
Si	2.21919100	-0.26340900	0.13903600
C	3.06964100	-1.96925700	0.29736300
H	3.87428100	-1.94785000	1.04697500
H	2.35324500	-2.74066400	0.60277000
H	3.51242000	-2.28503400	-0.65460800
C	3.52120300	1.01849800	-0.40963500
H	4.31779100	1.12299300	0.33971000
H	3.99434300	0.72864500	-1.35557500
H	3.07292100	2.00912200	-0.55193400
C	1.53596100	0.23874500	1.84244300
H	1.04801700	1.21929000	1.79781500
H	0.79623300	-0.48472200	2.20316000
H	2.33837400	0.30011500	2.58998200

C-5

C	-2.60040100	1.18675900	0.33951600
C	-1.46942300	0.54444100	-0.15833800
C	-1.46732800	-0.86768900	-0.44067600
C	-2.64903000	-1.61053400	-0.20761700
C	-3.77605400	-0.96052800	0.28703400
C	-3.75531400	0.41785500	0.55698700
H	-2.59404600	2.24987300	0.56160300

H	-2.66936200	-2.67673300	-0.41757500
H	-4.68575000	-1.52653700	0.46923100
H	-4.64742000	0.90127000	0.94592800
C	-0.20300000	-1.20129100	-0.93782100
C	0.67715500	0.01137900	-0.93812200
H	1.05009300	0.26323600	-1.95135000
N	-0.23553900	1.06630800	-0.46554900
H	0.12509100	-2.17898000	-1.26718700
Si	2.22663300	-0.25261000	0.21061400
C	1.63791900	-0.58572800	1.97362100
H	0.99268900	-1.46992600	2.01178500
H	2.48585400	-0.75559500	2.64815700
H	1.06176300	0.25931600	2.36736300
C	3.34849200	1.27776500	0.16942400
H	4.27698900	1.08485300	0.72148000
H	3.62963100	1.54587300	-0.85654600
H	2.87363300	2.15311200	0.62648200
C	3.19479900	-1.73099700	-0.47300900
H	3.49555400	-1.57050700	-1.51571500
H	4.10925300	-1.89888500	0.10902900
H	2.60495200	-2.65372400	-0.43396400
C	0.05601100	2.47889600	-0.51723300
H	0.26600400	2.90984200	0.47333100
H	0.92930700	2.64816300	-1.15325500
H	-0.79127900	3.02575500	-0.95113400

C-6

C	-2.94993700	-0.05238500	0.33372100
C	-1.70061400	0.38392400	-0.11407400
C	-0.69747000	-0.52654200	-0.51651700
C	-0.97197100	-1.88734800	-0.51168200
C	-2.23107500	-2.34083300	-0.08499700
C	-3.19975500	-1.42930500	0.33843700
H	-3.71024900	0.64905600	0.66404700
H	-0.22148600	-2.60184100	-0.84020100
H	-2.44791000	-3.40519100	-0.08017500
H	-4.16747000	-1.78994500	0.67769800
C	0.54803700	0.25353700	-0.89767700
C	0.12072800	1.67542200	-0.62610000
H	0.50957000	2.54398700	-1.14800600
N	-1.23180100	1.68341900	-0.26022900
C	-1.93278800	2.85708900	0.20493400
H	-2.98430600	2.81488900	-0.09850200
H	-1.88832000	2.96412300	1.29945500
H	-1.48084300	3.74437700	-0.24675600
H	0.81137900	0.08925500	-1.95933200
Si	2.12555300	-0.16622000	0.13485900
C	2.74940100	-1.91003300	-0.28081800
H	3.69682300	-2.11335800	0.23406400
H	2.03701300	-2.68308600	0.02859500
H	2.92854000	-2.03051900	-1.35636600
C	3.46907900	1.08675300	-0.33192600
H	4.39471300	0.89687600	0.22530200
H	3.71321200	1.03730200	-1.40041000
H	3.15112500	2.11144100	-0.10820200
C	1.72775000	-0.04724700	1.97888600
H	1.35545200	0.95153600	2.23282200
H	0.96018800	-0.77407100	2.26813200
H	2.61911900	-0.23987400	2.58829500

TS-8

H	2.06761600	-0.97560200	-0.78352300
Si	4.31137300	-2.00057400	0.50095100

C	5.14948900	-3.04714800	-0.85040700
H	5.54813100	-3.96726300	-0.40335700
H	5.99740700	-2.52301600	-1.30746400
H	4.46318300	-3.34203100	-1.65131000
C	3.04035500	-3.12060800	1.37597700
H	3.52766500	-3.98447300	1.84489200
H	2.30417700	-3.50055600	0.65559300
H	2.50436500	-2.57799200	2.16540200
C	5.66557200	-1.52411100	1.74580500
H	5.24256500	-0.97813100	2.59674600
H	6.40843300	-0.86719200	1.27666400
H	6.19606400	-2.40310600	2.13410700
O	0.94564100	-1.21732500	-1.11045200
C	0.77620800	-1.59224900	-2.47085500
C	-0.45457200	-2.51817800	-2.56716800
H	-1.32359800	-2.10836500	-2.03875300
H	-0.23362400	-3.48715900	-2.10056100
H	-0.73465900	-2.71693200	-3.61080700
C	0.56707000	-0.32653400	-3.33041400
H	1.44772500	0.32206900	-3.26858200
H	-0.28276400	0.26291500	-2.95908200
H	0.39079300	-0.56271800	-4.38831600
C	1.98915300	-2.37387400	-3.01004500
H	2.89102900	-1.75879600	-3.01276900
H	1.80930800	-2.71583600	-4.03710600
H	2.17692600	-3.25435500	-2.38614300
K	0.07288900	1.50333200	0.19465800
C	3.73699700	1.77908100	-0.53585500
C	3.04622200	1.69371700	0.72530200
C	2.83227200	0.32930500	0.98148700
C	3.34016000	-0.49370300	-0.12301900
H	2.35654700	-0.07694400	1.86746800
O	-1.06016000	0.17284100	2.22463300
K	-0.74705800	-2.00909800	0.82667900
C	-0.92169500	0.17322700	3.60716100
C	0.09121100	1.24928900	4.06920000
H	0.20351100	1.28836800	5.16109900
H	1.07777400	1.05029500	3.63523500
H	-0.23555200	2.23972300	3.72609500
C	-2.27873900	0.46896700	4.30793000
H	-3.02773500	-0.28881200	4.03228400
H	-2.20318500	0.46809000	5.40306100
H	-2.65084900	1.46006500	4.00879800
C	-0.42599400	-1.20913400	4.11332100
H	0.53967400	-1.45281700	3.64974000
H	-0.28933400	-1.24651800	5.20206800
H	-1.15061800	-1.99339800	3.84637600
O	-2.42925500	1.96079300	-0.83149100
O	-3.21993800	-1.54870200	-0.27586700
K	-3.40223100	0.64793500	1.24117000
K	-2.99084500	-0.01527700	-2.33575800
C	-4.16792700	-2.56287000	-0.21810700
C	-3.53049500	-3.89985600	0.24672300
H	-3.11305600	-3.78687300	1.25782000
H	-4.24943600	-4.72861600	0.28351200
H	-2.72120900	-4.18964900	-0.43681200
C	-4.81274900	-2.80266200	-1.61102900
H	-5.55659500	-3.60990400	-1.60962800
H	-5.32698200	-1.89098700	-1.95229400
H	-4.03832000	-3.06401100	-2.34511000
C	-5.30357400	-2.20454700	0.77779200
H	-4.88784900	-2.05223500	1.78360300
H	-5.80189200	-1.27596100	0.46310100

H	-6.07381400	-2.98334400	0.85221100
C	-2.79111800	3.26207900	-1.16344200
C	-3.30108200	3.33836000	-2.62878500
H	-4.19298000	2.70468600	-2.75492500
H	-3.58142100	4.35396500	-2.93650800
H	-2.51937600	2.98683800	-3.31695600
C	-3.92808400	3.76828800	-0.23536500
H	-3.59011700	3.76107400	0.81040300
H	-4.25351700	4.79029300	-0.46969600
H	-4.80604700	3.11137300	-0.32190900
C	-1.58920600	4.23009000	-1.02480600
H	-1.84095300	5.26505600	-1.29043300
H	-1.22573300	4.23687900	0.01194500
H	-0.76576700	3.91012300	-1.67733900
N	4.01226100	0.50195800	-0.96710000
C	4.57599000	0.25512200	-2.27037600
H	5.47408600	0.86848200	-2.41488000
H	4.86538300	-0.79237500	-2.35842800
H	3.87612900	0.49357500	-3.09036900
C	2.68709200	2.90503400	1.38043600
C	4.01482400	3.00311400	-1.14404100
C	3.64353300	4.18657700	-0.46706500
H	3.86825300	5.15004200	-0.91707400
C	2.99951600	4.13054500	0.77358100
H	2.73885700	5.05609500	1.28294800
H	4.52688100	3.05491600	-2.10081900
H	2.21421900	2.87962700	2.35975100
TS-9			
H	2.01042500	-0.68328700	-0.78720500
Si	4.03929400	-2.20834300	0.08301900
C	4.92618100	-2.67837200	-1.52945800
H	5.31733000	-3.70115400	-1.45173000
H	5.78055000	-2.01848200	-1.72065600
H	4.27076400	-2.64066500	-2.40541900
C	2.68768800	-3.51443100	0.41521500
H	3.11463100	-4.51225100	0.57705100
H	2.00031700	-3.57687200	-0.43886100
H	2.10340600	-3.25598300	1.30864400
C	5.33134100	-2.35619800	1.47366500
H	4.89037700	-2.16199100	2.45867000
H	6.14059200	-1.62964900	1.32895400
H	5.78308700	-3.35618400	1.50196000
O	0.90053200	-0.76319400	-1.27169100
C	0.82073700	-0.49544600	-2.66556400
C	-0.41570300	-1.23184000	-3.22430400
H	-1.31340400	-1.05758200	-2.61868700
H	-0.24168400	-2.31597400	-3.21770700
H	-0.62533000	-0.94546000	-4.26444500
C	0.69974300	1.02794000	-2.89537100
H	1.60596500	1.53166900	-2.54085000
H	-0.14414000	1.44766000	-2.32953200
H	0.56769300	1.28081100	-3.95611500
C	2.05596600	-1.01326500	-3.42272600
H	2.95936900	-0.49416300	-3.09613000
H	1.94710700	-0.85818900	-4.50376400
H	2.18482800	-2.08626400	-3.24424100
K	0.07791000	1.12966800	0.76855400
C	3.70555500	1.77338500	0.44954800
C	2.70163800	-0.07979200	1.38008000
C	3.22431600	-0.51473900	0.05828700
H	2.73217600	-0.67524000	2.29298400
O	-1.34954300	-0.68180800	2.14109300

K	-0.97144100	-2.18792000	0.04587500
C	-1.26547400	-1.14840800	3.44495800
C	-0.24713300	-0.31771800	4.26565200
H	-0.15798700	-0.65323400	5.30780500
H	0.74188800	-0.38476300	3.79762700
H	-0.55153400	0.73793700	4.27400200
C	-2.64320400	-1.05986200	4.16028700
H	-3.39434400	-1.64766700	3.61230000
H	-2.61737500	-1.43710000	5.19105200
H	-2.97987600	-0.01330000	4.20551500
C	-0.81381400	-2.63353100	3.47117300
H	0.16444500	-2.73366200	2.98228700
H	-0.72261000	-3.04024400	4.48715800
H	-1.54037500	-3.25807400	2.93017900
O	-2.28792800	2.24313300	-0.08923200
O	-3.33390000	-1.12429900	-0.95524700
K	-3.53524800	0.33919800	1.26607300
K	-2.88244600	1.05931000	-2.26200700
C	-4.32351000	-2.01621800	-1.34777700
C	-3.78417400	-3.47142700	-1.38543900
H	-3.45441400	-3.77735100	-0.38194600
H	-4.53548600	-4.20029100	-1.71614400
H	-2.92924200	-3.53825900	-2.07162200
C	-4.85458100	-1.67012000	-2.76628300
H	-5.62575200	-2.36585200	-3.12148900
H	-5.30241900	-0.66424700	-2.76796600
H	-4.02952400	-1.68767600	-3.49144700
C	-5.52554500	-1.97815400	-0.36562000
H	-5.19199800	-2.24443800	0.64702400
H	-5.95492800	-0.96602500	-0.33527700
H	-6.33187600	-2.67048000	-0.64154300
C	-2.49596900	3.59962400	0.12791500
C	-2.93016600	4.31146400	-1.18274600
H	-3.87196900	3.87899000	-1.55437900
H	-3.09700800	5.38892100	-1.05501600
H	-2.15710500	4.18478600	-1.95357800
C	-3.61102200	3.82328400	1.18507800
H	-3.32380600	3.35700800	2.13799700
H	-3.81174400	4.88436600	1.38335800
H	-4.55095700	3.36545300	0.84368700
C	-1.20482000	4.28964300	0.64019000
H	-1.33118700	5.36793000	0.80302700
H	-0.89648700	3.84849000	1.59877100
H	-0.39051800	4.15414000	-0.08419700
C	3.91525700	0.69361000	-0.45286800
C	4.65595600	0.95271900	-1.61464700
C	4.19144000	3.05752400	0.20806600
C	4.91637700	3.28570600	-0.97177100
C	5.14840100	2.24237600	-1.86802900
H	4.87872300	0.15103900	-2.31276300
H	5.72878600	2.42405800	-2.76949500
H	5.31081800	4.27810500	-1.17452200
H	4.03019700	3.86434100	0.91880300
N	2.94529400	1.32233800	1.54028000
C	3.09352900	1.90879800	2.85974800
H	4.07922500	1.68845300	3.30343500
H	2.97136900	2.99571500	2.81441800
H	2.31973800	1.50777900	3.52144900
C-10			
C	-2.82273700	1.23418200	0.00976200
C	-1.63506300	0.48908600	0.01279800
C	-1.63870700	-0.93288900	-0.00152300

C	-2.86940700	-1.61371600	-0.00662500
C	-4.04690500	-0.87869600	-0.00384300
C	-4.02229900	0.53220100	0.00336000
H	-2.81419400	2.32048200	0.00854400
H	-2.89529300	-2.70063600	-0.01484200
H	-5.00410600	-1.39315000	-0.00914100
H	-4.96011300	1.08141800	0.00134300
C	-0.26641300	-1.33605200	-0.00689900
C	0.52772400	-0.20361500	0.00597000
N	-0.32094700	0.91168700	0.02837100
H	0.09957700	-2.35419000	-0.01289000
C	0.06904200	2.30607600	-0.02114600
H	-0.52580900	2.88784100	0.69116500
H	1.11866300	2.40710200	0.25663500
H	-0.07130900	2.73328700	-1.02298500
Si	2.41292200	-0.19564600	0.00091100
C	3.08569000	0.71763200	-1.51892700
H	2.80762400	1.77773100	-1.53539700
H	4.18158100	0.66688300	-1.54298600
H	2.71200400	0.26383600	-2.44424200
C	2.97746600	-1.99929200	-0.06594400
H	4.07288700	-2.05309700	-0.07503400
H	2.62637700	-2.56823100	0.80238300
H	2.61450500	-2.50467900	-0.96798000
C	3.09981200	0.60248700	1.57891100
H	2.72299500	0.08904600	2.47110000
H	4.19509600	0.53688900	1.59430800
H	2.83602200	1.66228600	1.67329700

C-11

C	-3.16143900	-0.16430600	-0.00035300
C	-1.85789700	0.34417000	0.00152100
C	-0.70717800	-0.49234700	0.00238600
C	-0.89640300	-1.88517900	0.00244800
C	-2.18822100	-2.39886800	0.00045200
C	-3.31039800	-1.54714100	-0.00110400
H	-4.02757300	0.49193300	-0.00161700
H	-0.04250500	-2.55811400	0.00342400
H	-2.33818500	-3.47520900	-0.00033700
H	-4.30853100	-1.97675600	-0.00320900
C	0.46433900	0.36553400	0.00156900
C	-0.03964300	1.64888000	0.00066500
H	0.49048700	2.59313000	-0.00117000
N	-1.42019700	1.65655300	0.00120000
C	-2.27216400	2.82695300	0.00080800
H	-2.91106600	2.84901200	-0.89029000
H	-2.91313200	2.84762400	0.89044500
H	-1.64660700	3.72230000	0.00230900
Si	2.27593500	-0.09709100	0.00046200
C	2.67291600	-1.18726400	-1.49934700
H	3.72752800	-1.49012200	-1.50243100
H	2.06603700	-2.10039600	-1.50832700
H	2.47501000	-0.65426600	-2.43685100
C	2.72192400	-1.03683100	1.58554100
H	3.77708800	-1.33776000	1.58529000
H	2.55109900	-0.41584200	2.47284600
H	2.11799100	-1.94464800	1.70062900
C	3.31410100	1.48702800	-0.09269500
H	3.13415700	2.14480000	0.76628800
H	4.38391200	1.24490500	-0.09905300
H	3.10296300	2.05903000	-1.00416000

C-9

O	-1.72862800	1.86541700	-0.20460500
O	1.39375500	-0.03456600	1.19272200
O	2.62894700	-0.07035200	-1.10788600
O	-1.75413400	-1.81702100	-0.32105800
K	-1.42164200	-0.02917500	1.52773000
K	0.83640100	2.02648900	-0.59193800
K	-2.34181700	0.09170700	-2.10200600
K	0.80406000	-2.04871700	-0.72157500
C	-2.49771800	3.00269600	0.01696300
C	2.00649600	-0.16441600	2.44790100
C	-2.55192600	-2.94505100	-0.16365200
C	-3.70083000	3.06028300	-0.95991200
H	-4.33265200	2.16968500	-0.83033500
H	-4.33586300	3.94244600	-0.80439900
H	-3.34321200	3.08516700	-1.99820400
C	-1.65626200	4.29103200	-0.18649200
H	-2.23723000	5.21154800	-0.04207600
H	-0.82009100	4.31697300	0.52899400
H	-1.24587200	4.31127700	-1.20567500
C	-3.05518300	3.01644500	1.46602600
H	-3.69100300	2.13484700	1.63310200
H	-2.22703900	2.99103800	2.18911600
H	-3.66079700	3.90569700	1.68569900
C	3.09787800	0.91655300	2.63894700
H	2.65423800	1.91780200	2.55593300
H	3.59417600	0.84721700	3.61550700
H	3.86970400	0.82416600	1.86612300
C	2.65235400	-1.56458100	2.59427400
H	3.15055200	-1.70321500	3.56273700
H	1.88285600	-2.34350100	2.50028600
H	3.39808400	-1.72686200	1.80706400
C	0.98085000	0.00292900	3.59890500
H	0.23634200	-0.80633600	3.58140300
H	1.45839000	-0.03094100	4.58585100
H	0.46615600	0.97060900	3.51670200
C	-3.72559300	-2.94124800	-1.17691200
H	-3.33543500	-2.92356400	-2.20354900
H	-4.37773200	-3.81959600	-1.08153100
H	-4.34920300	-2.04817700	-1.02602500
C	-1.73191700	-4.24390100	-0.38960900
H	-0.91093000	-4.30767900	0.34079300
H	-2.33380100	-5.15611900	-0.28368800
H	-1.30268800	-4.24455900	-1.40141300
C	-3.15217400	-3.00080700	1.26739500
H	-2.34566600	-3.02533800	2.01475000
H	-3.77078200	-2.11035800	1.45070200
H	-3.78539400	-3.88218300	1.43473400
C	3.99651900	0.09333800	-1.53082800
C	4.00201700	-0.19621100	-3.03531300
H	3.67723000	-1.22499700	-3.23007700
H	3.31482400	0.47727200	-3.55905600
H	5.00622700	-0.06555800	-3.45438700
C	4.45316400	1.53895300	-1.26663700
H	3.82860600	2.24583400	-1.82817700
H	4.38829700	1.78514100	-0.19992900
H	5.49185400	1.69194700	-1.58262800
C	4.90343800	-0.90199300	-0.79126100
H	4.91735300	-0.70398600	0.28636400
H	4.55058800	-1.92847500	-0.94837500
H	5.93505100	-0.83886000	-1.15663000
H	2.47564000	-0.03610500	-0.10388600

C	0.17519000	1.11963000	-0.01485600
C	1.49171700	0.71186000	0.01656000
C	1.49173400	-0.71185300	0.01655100
C	0.17519800	-1.11962700	-0.01486200
N	-0.62562000	-0.00000800	-0.04101500
H	2.35599000	-1.36255500	0.02288100
C	-2.07410700	-0.00000300	0.02737100
H	-2.46519000	0.88644200	-0.47969900
H	-2.46519100	-0.88640900	-0.47976900
H	-2.43439200	-0.00004100	1.06388200
H	2.35596300	1.36257800	0.02294300
H	-0.26313000	2.10801400	-0.02389800
H	-0.26310400	-2.10801700	-0.02381900

TS-10

C	-0.92038000	-0.13975800	-0.97230800
C	-1.29152400	-1.46617800	-0.64010700
C	-2.24015700	-1.39697800	0.39975100
C	-2.51401000	-0.05744100	0.62498600
N	-1.78769100	0.70021000	-0.26437200
H	-2.69644400	-2.22775100	0.92173500
C	-1.66534400	2.13986800	-0.23539500
H	-1.63704500	2.53872400	-1.25485200
H	-2.52919300	2.56793100	0.27913100
H	-0.74577600	2.44880000	0.28301600
H	-0.88425200	-2.35972300	-1.09343200
H	-0.55905300	0.19568300	-1.93779300
H	-3.17379000	0.41604800	1.33903100
Si	1.42961200	0.03307300	0.05649700
C	2.28491700	-1.14050900	-1.17881300
H	3.29724700	-1.39797000	-0.83889600
H	1.72871500	-2.07737000	-1.29742700
H	2.37980800	-0.68191400	-2.17092800
C	2.52291900	1.60066700	0.20426500
H	3.54710500	1.34075300	0.51065000
H	2.59169600	2.13457000	-0.75101300
H	2.12345200	2.30060500	0.94766700
C	1.33888500	-0.80848700	1.76078400
H	0.98341300	-0.11471900	2.53127800
H	0.65366200	-1.66204800	1.74109100
H	2.32789600	-1.17322200	2.07140900

TS-11

C	1.32882700	-0.47665600	-1.01496500
C	0.43058400	0.60843600	-1.17976200
C	1.01755100	1.69891400	-0.40763400
C	2.08670100	1.19826300	0.27823000
N	2.28377500	-0.12327300	-0.08100100
H	0.64082800	2.71098800	-0.34630600
C	3.21686000	-1.03371500	0.54683100
H	3.60661400	-1.73593500	-0.19739700
H	4.05704000	-0.46743300	0.95792500
H	2.74929100	-1.60853800	1.35821800
H	-0.10580300	0.76733700	-2.10898700
H	1.31682500	-1.46899600	-1.44187600
H	2.74400000	1.66764000	0.99820900
Si	-1.61108900	-0.05338400	0.03940300
C	-2.19728400	-1.63621500	-0.85019200
H	-2.91097900	-2.20308300	-0.23688500
H	-2.69228200	-1.40095700	-1.80015400
H	-1.35376300	-2.30144300	-1.07099300
C	-0.91378700	-0.53267800	1.74317400
H	-1.66572400	-1.05414500	2.35016000

H	-0.05045200	-1.20028600	1.63899000
H	-0.58550600	0.35040500	2.30280300
C	-3.11746600	1.09699700	0.30530700
H	-2.82143000	2.02320000	0.81208600
H	-3.58120400	1.37582200	-0.64830400
H	-3.89055900	0.61564700	0.92193600

C-13

C	-0.46405100	-0.13238300	-0.69391800
C	-1.00830200	-1.53540700	-0.62642400
C	-2.21136200	-1.51811600	0.06553200
C	-2.50355300	-0.21270800	0.44611400
N	-1.46548800	0.64665800	0.08139200
H	-2.83001700	-2.37841500	0.29373700
C	-1.75783400	2.00723100	-0.32802700
H	-2.17791800	2.05965700	-1.34811500
H	-2.48333500	2.44671800	0.36412000
H	-0.84996800	2.61702000	-0.29986700
H	-0.51654000	-2.39630600	-1.06050400
H	-0.42961600	0.24823500	-1.73749900
H	-3.34871500	0.16971200	1.00386500
Si	1.31164200	0.00030100	0.06087100
C	2.46415100	-1.08023400	-0.98843900
H	3.49569700	-1.02626500	-0.61915800
H	2.16187100	-2.13368400	-0.96647000
H	2.47413800	-0.75845300	-2.03718800
C	1.93271400	1.79270700	-0.00102900
H	2.97583700	1.85107400	0.33435400
H	1.89177700	2.20263400	-1.01764400
H	1.34409000	2.44875100	0.65068400
C	1.27857700	-0.60383300	1.85057500
H	0.58811900	-0.00123100	2.45124200
H	0.94578000	-1.64582700	1.90999700
H	2.27217700	-0.53798300	2.31021600

C-14

C	1.17431500	-0.73147200	-0.64577200
C	0.11670500	0.32239300	-0.84870400
C	0.80956100	1.55673700	-0.30576100
C	2.06301000	1.23231400	0.07083600
N	2.34143400	-0.10569500	-0.19401500
H	0.37200200	2.54540700	-0.25524300
C	3.47197500	-0.82520300	0.34702300
H	3.75188200	-1.63678200	-0.33407300
H	4.32701500	-0.14912300	0.44156500
H	3.25679200	-1.26539300	1.33319700
H	-0.15971300	0.45032700	-1.91693600
H	1.27085300	-1.64175400	-1.22881500
H	2.83093900	1.85636500	0.51329700
Si	-1.52180300	-0.11397600	0.07148000
C	-2.18797300	-1.74514000	-0.62792100
H	-3.12135300	-2.04177600	-0.13372300
H	-2.39480800	-1.66580200	-1.70238900
H	-1.46507000	-2.55705500	-0.48630900
C	-1.19224400	-0.28435700	1.92593900
H	-2.10787000	-0.53843300	2.47371200
H	-0.45367600	-1.07106800	2.11708300
H	-0.79756900	0.64915700	2.34317400
C	-2.79104900	1.26459100	-0.23445100
H	-2.44533900	2.22589000	0.16446400
H	-2.98474000	1.40060900	-1.30566800
H	-3.74993700	1.03577700	0.24691200

TS-12

H	2.33008500	0.09525700	-0.79600000
Si	4.83774000	-1.00449100	-0.24871300
C	5.80867300	-0.74709600	-1.86488300
H	6.46697500	-1.60873300	-2.03646300
H	6.45291800	0.13877800	-1.80631300
H	5.16941000	-0.64091700	-2.74707900
C	3.89258100	-2.65480200	-0.37113000
H	4.57249900	-3.49379400	-0.56468400
H	3.15404600	-2.62207900	-1.18162400
H	3.36159500	-2.87389900	0.56503500
C	6.13573200	-1.16002800	1.13084700
H	5.66369000	-1.39487300	2.09165700
H	6.67796900	-0.21495800	1.25820400
H	6.87413700	-1.94247800	0.91354200
O	1.27504200	-0.16452100	-1.24464100
C	1.09285400	0.11077000	-2.63163400
C	0.11001800	-0.93448300	-3.20070100
H	-0.80854900	-1.00962700	-2.60577100
H	0.57455200	-1.92936000	-3.19648800
H	-0.16419200	-0.70665700	-4.24074500
C	0.52355700	1.53653200	-2.80642200
H	1.27287300	2.28392200	-2.51873500
H	-0.34274300	1.70169000	-2.15341000
H	0.23273500	1.74269000	-3.84684000
C	2.41095800	-0.00380800	-3.41702100
H	3.14362400	0.72576800	-3.06450100
H	2.24342600	0.17258900	-4.48719900
H	2.83953900	-1.00476400	-3.29976700
K	0.20263500	1.46011400	0.87189800
C	3.55137600	2.39117800	1.26494000
C	3.01501900	1.44356700	2.14017500
C	3.01518200	0.20334900	1.50029900
C	3.55311400	0.34090200	0.13580300
H	2.68069600	-0.73093000	1.93658800
O	-0.86243800	-0.63881800	2.17266600
K	-0.26758200	-2.00338900	0.03184000
C	-0.70947800	-1.13702700	3.45926500
C	0.08822400	-0.14853000	4.34519200
H	0.22113000	-0.50571500	5.37530200
H	1.08025000	0.02030400	3.91206000
H	-0.43411500	0.81697700	4.38498300
C	-2.08982300	-1.37695200	4.13415400
H	-2.68806500	-2.08255300	3.53894400
H	-2.00579400	-1.79002800	5.14791700
H	-2.64163600	-0.42844900	4.21573100
C	0.04512000	-2.49468600	3.44028100
H	1.03056200	-2.36875700	2.97204800
H	0.20435200	-2.91465200	4.44220500
H	-0.52519900	-3.23605000	2.86038500
O	-2.35044600	2.02837700	-0.08033500
O	-2.79572800	-1.49174700	-0.90121900
K	-3.21213700	-0.05020500	1.31125400
K	-2.85565500	0.72477000	-2.22970900
C	-3.58994300	-2.57753800	-1.24830800
C	-2.77069600	-3.89619100	-1.23892900
H	-2.37787900	-4.08933000	-0.23010800
H	-3.36337600	-4.77310100	-1.52996700
H	-1.92628000	-3.81810600	-1.93728300
C	-4.18563500	-2.39983100	-2.67174400
H	-4.79776300	-3.25230000	-2.99380100
H	-4.83129300	-1.50868600	-2.70549800
H	-3.37667200	-2.27251700	-3.40376700

C	-4.76933800	-2.74077800	-0.25209700
H	-4.38413100	-2.90091500	0.76468700
H	-5.38771300	-1.83129600	-0.24942700
H	-5.42590900	-3.58665800	-0.49482900
C	-2.80738600	3.32632700	0.11527300
C	-3.36464700	3.92482900	-1.20561400
H	-4.21295500	3.32257600	-1.56705700
H	-3.72595500	4.95543000	-1.09441200
H	-2.58239100	3.92704100	-1.97706300
C	-3.94598900	3.35765700	1.17063200
H	-3.58039000	2.96457600	2.12971600
H	-4.33722400	4.36703900	1.35449100
H	-4.78702500	2.73224500	0.83671800
C	-1.66747600	4.25363500	0.61240200
H	-1.98858600	5.29527500	0.74338400
H	-1.28989100	3.90525200	1.58456100
H	-0.83588400	4.24708500	-0.10500600
N	4.02505500	1.73545100	0.13036500
C	4.25649700	2.47466300	-1.08690600
H	4.81654800	3.38893700	-0.86049400
H	4.84618600	1.87985500	-1.78778500
H	3.31464000	2.77330400	-1.58991100
H	2.67885400	1.65417300	3.15028900
H	3.81422600	3.42533400	1.44760800
TS-13			
H	2.25007300	-0.31785000	-0.87102600
Si	4.53129900	-1.40151500	0.02357900
C	5.45218900	-1.88293000	-1.56686300
H	6.08171600	-2.76416400	-1.38883300
H	6.11245800	-1.07113000	-1.89606800
H	4.77849700	-2.11761500	-2.39697500
C	3.38480400	-2.84908900	0.51868300
H	3.95187800	-3.76255300	0.73819900
H	2.68133700	-3.07424400	-0.29341600
H	2.80818100	-2.59920000	1.42084800
C	5.84951900	-1.23655300	1.38808900
H	5.39195700	-1.05540800	2.36814300
H	6.51596200	-0.39069300	1.17967000
H	6.46943500	-2.13925000	1.46908000
O	1.17369900	-0.61670200	-1.27500800
C	1.01983200	-0.54999200	-2.69001800
C	-0.02521800	-1.61003900	-3.09391600
H	-0.92726800	-1.54680400	-2.47220600
H	0.38524600	-2.61678300	-2.94411100
H	-0.31133200	-1.52590000	-4.15106900
C	0.55706700	0.86607500	-3.09366000
H	1.33013100	1.59421700	-2.81539600
H	-0.36394600	1.15597600	-2.56829800
H	0.38138600	0.95567600	-4.17381500
C	2.33600400	-0.86136800	-3.42293200
H	3.10429200	-0.12877100	-3.16120700
H	2.19205600	-0.83687800	-4.51049300
H	2.69514500	-1.85930300	-3.15074800
K	0.23887200	1.56702200	0.32019800
C	3.48966800	2.13159800	1.06761500
C	3.13057000	0.81782500	1.08289100
C	3.50456900	0.16717200	-0.19219200
H	2.69380000	0.31529000	1.94017200
O	-0.65620400	-0.12302000	2.20550900
K	-0.27570700	-2.03872900	0.46615800
C	-0.38989200	-0.16799100	3.56780400
C	0.29473500	1.13942000	4.04428300

H	0.49775200	1.14835600	5.12362300
H	1.24852400	1.28121300	3.52185300
H	-0.34899400	1.99932200	3.81388800
C	-1.69921000	-0.34132600	4.38944900
H	-2.23397600	-1.24484700	4.06296000
H	-1.51851400	-0.43303900	5.46840600
H	-2.35938500	0.52816300	4.24819900
C	0.53913600	-1.36280400	3.90975800
H	1.47745500	-1.28217500	3.34644400
H	0.79128400	-1.42150600	4.97691200
H	0.05255100	-2.30987800	3.63286900
O	-2.37769900	1.96760000	-0.44372700
O	-2.83967600	-1.65353400	-0.42283200
K	-3.09152600	0.24901400	1.43501000
K	-2.91695200	0.21023200	-2.21048300
C	-3.68084300	-2.75696300	-0.48629600
C	-2.89863000	-4.07312800	-0.23063400
H	-2.45377200	-4.05801500	0.77498000
H	-3.53030500	-4.96869200	-0.29277700
H	-2.09343700	-4.18120900	-0.97016400
C	-4.35106300	-2.86714700	-1.88348900
H	-5.00251400	-3.74504100	-1.98308300
H	-4.97449500	-1.98038200	-2.07641200
H	-3.58133000	-2.93124200	-2.66455900
C	-4.80684100	-2.65482500	0.57759200
H	-4.36978300	-2.60925600	1.58500700
H	-5.39599000	-1.74080900	0.41351200
H	-5.50162300	-3.50482100	0.55669400
C	-2.85459200	3.27170000	-0.50598400
C	-3.48633000	3.56491700	-1.89437100
H	-4.33803000	2.89008300	-2.07321100
H	-3.86237100	4.59176300	-1.99050600
H	-2.74112200	3.40742200	-2.68625200
C	-3.94272100	3.51246600	0.57508700
H	-3.52135500	3.34449400	1.57630100
H	-4.35209000	4.53104700	0.55647200
H	-4.78045300	2.81487300	0.42878200
C	-1.71437000	4.29704000	-0.27432100
H	-2.05674900	5.33873600	-0.32947900
H	-1.27104400	4.15075500	0.72104000
H	-0.92629500	4.16519900	-1.02803100
H	3.38868900	2.88891400	1.83737200
N	4.16856900	2.42848700	-0.11843600
C	4.22348000	3.77342400	-0.64425100
H	5.00653300	3.84013200	-1.40566100
H	3.26386900	4.07545200	-1.11400600
H	4.46239600	4.47969700	0.15771400
C	4.04727500	1.29984800	-0.96821900
H	4.77055800	1.22050300	-1.77535200
C-15			
C	2.76920200	-0.03748400	0.01656200
C	2.59736300	1.33036400	-0.00508000
C	1.19935600	1.56227900	-0.01550400
C	0.53719200	0.33584900	0.00015800
N	1.53459400	-0.63672800	0.02456600
H	0.71253700	2.52888300	-0.02626400
C	1.33335500	-2.07396200	-0.01761500
H	2.28230200	-2.57179400	0.19551800
H	0.60681100	-2.38620700	0.73863300
H	0.98140700	-2.40318700	-1.00232300
Si	-1.31928000	0.06950000	0.00151200
C	-1.88075600	-0.96583500	-1.48687500

H	-1.47502700	-1.98407100	-1.46859800
H	-2.97468400	-1.05232200	-1.50425600
H	-1.56899900	-0.50149800	-2.42977700
C	-2.12763800	1.77728600	-0.10624900
H	-3.22031900	1.68190600	-0.10667500
H	-1.85211700	2.41192500	0.74375100
H	-1.84029800	2.30290900	-1.02393400
C	-1.90621100	-0.78052000	1.59420400
H	-1.60031500	-0.20997800	2.47879100
H	-3.00093100	-0.85739600	1.60858900
H	-1.50925300	-1.79684100	1.70263900
H	3.38590600	2.07105500	-0.00530700
H	3.66956100	-0.63715700	0.02846800

C-16

Si	1.61223500	0.09240300	0.00204100
C	2.40598100	-0.67347600	1.54497300
H	3.49264300	-0.52116600	1.55202400
H	1.99929500	-0.22876400	2.46092000
H	2.22334600	-1.75375200	1.59544500
C	2.41146900	-0.67456800	-1.53761000
H	3.49787200	-0.52008000	-1.54221600
H	2.23095900	-1.75525900	-1.58664200
H	2.00621400	-0.23224000	-2.45534900
C	1.93424400	1.96149300	0.00128300
H	1.51213500	2.44573700	-0.88757500
H	1.50277500	2.44797500	0.88437800
H	3.01152600	2.16802700	0.00652300
C	-2.27128400	-1.23540500	-0.00974300
C	-0.91856400	-1.48082400	0.01005700
C	-0.22963500	-0.21921400	0.00168700
H	-3.11871600	-1.90751000	-0.01154800
H	-0.46269800	-2.46304100	0.01612300
C	-3.74295300	0.80441200	0.02836600
H	-4.47751700	0.26407600	-0.57601500
H	-4.11594800	0.87310900	1.05784900
H	-3.64115000	1.81486300	-0.37574800
N	-2.46001800	0.13008300	-0.03463900
C	-1.23054100	0.74133600	-0.02109700
H	-1.16419700	1.82126600	-0.03177000

C-17

C	1.09505600	-0.34701200	0.00013900
C	0.71743600	0.96026000	0.00021000
C	-0.71827600	0.95974100	-0.00004800
C	-1.09464700	-0.34795700	-0.00019000
H	-1.37495200	1.81859400	-0.00009300
H	1.37344000	1.81964700	0.00039800
H	2.05048400	-0.84907400	0.00024400
O	0.00042800	-1.16109700	-0.00010500
H	-2.04980900	-0.85058400	-0.00037400

TS-14

C	2.53815600	-0.82127300	0.28585000
C	2.59945200	0.50728700	0.59970200
C	1.73544900	1.17783000	-0.31070700
C	1.12797600	0.18819300	-1.07754400
H	1.54378800	2.23989500	-0.37481900
H	3.19869500	0.95110900	1.38311400
H	3.01185700	-1.70309900	0.68986400
O	1.69841300	-1.03150100	-0.76971500
H	0.69533100	0.24590500	-2.06531600
Si	-1.32380600	-0.04012700	0.01138400

C	-2.04297300	1.69414700	-0.31108200
H	-2.97321000	1.84719700	0.25325000
H	-1.34009800	2.47834900	-0.00667700
H	-2.27270900	1.84476300	-1.37259100
C	-2.56298900	-1.36202200	-0.58534500
H	-3.51842600	-1.28382200	-0.04657700
H	-2.77673900	-1.25779800	-1.65537800
H	-2.17075700	-2.37216900	-0.42169500
C	-1.00201700	-0.26045500	1.87194800
H	-0.67055900	-1.27967900	2.09987100
H	-0.22605700	0.42785600	2.22350700
H	-1.91346600	-0.06696400	2.45485600

TS-15

C	-2.52511800	-0.79798700	0.23107900
C	-1.65488000	-1.08140300	-0.76219800
C	-0.97714000	0.16930200	-1.10141500
C	-1.65185300	1.13425100	-0.34708500
H	-0.53362900	0.37941200	-2.06696500
H	-1.45317200	-2.05788700	-1.18048400
H	-3.19585700	-1.40415000	0.82189600
O	-2.52983700	0.54070400	0.52784000
H	-1.54852000	2.20365400	-0.25167100
Si	1.29292300	-0.04291400	-0.00596500
C	1.97677100	1.72701900	-0.16250000
H	2.84538500	1.87784000	0.49267100
H	2.29560400	1.94557200	-1.18868900
H	1.22106000	2.46989800	0.11811300
C	0.80499300	-0.38652800	1.79657800
H	1.64238800	-0.18934300	2.47913300
H	-0.03466400	0.24626200	2.10519500
H	0.50117900	-1.43031900	1.93392600
C	2.63530100	-1.28623100	-0.55464600
H	2.26936100	-2.31790300	-0.49694900
H	2.95227500	-1.10290100	-1.58789300
H	3.52791700	-1.21550300	0.08364100

C-18

C	2.50125300	-0.71926400	0.16369400
C	2.61622000	0.65784800	0.20646500
C	1.48406900	1.20959100	-0.38332600
C	0.59097400	0.08424400	-0.80689400
H	1.26564600	2.25756900	-0.53914500
H	3.45708800	1.19649900	0.62593200
H	3.14795500	-1.51140300	0.51306400
O	1.33874900	-1.12298600	-0.43537900
H	0.44280800	0.04194500	-1.90182700
Si	-1.13924800	0.00406500	0.05700700
C	-2.08691500	1.57679700	-0.41119100
H	-3.09274400	1.57214900	0.02637700
H	-1.57586300	2.47728100	-0.05068400
H	-2.20293200	1.67035800	-1.49788800
C	-2.05185500	-1.52617600	-0.57817800
H	-3.02854500	-1.63848600	-0.09171200
H	-2.22504500	-1.47107900	-1.65976100
H	-1.47171200	-2.43448300	-0.38024500
C	-0.88471000	-0.09598500	1.92529800
H	-0.32122600	-0.99609200	2.19488300
H	-0.32566900	0.77045100	2.29584200
H	-1.84448800	-0.13006400	2.45488400

C-19

C	2.53696700	0.67415000	0.18742900
---	------------	------------	------------

C	1.45858300	1.17234000	-0.42624500
C	0.57107000	0.02412300	-0.85447300
C	1.45602400	-1.13606900	-0.50322300
H	0.33908800	0.06066400	-1.93555100
H	1.24279100	2.22245300	-0.57326800
H	3.38923300	1.15347900	0.65029900
O	2.55861500	-0.70143700	0.22647100
H	1.16156900	-2.15298700	-0.27270700
Si	-1.14429500	0.00480700	0.04990800
C	-2.09545400	-1.53257300	-0.51792600
H	-3.08292700	-1.58230600	-0.04289200
H	-2.25169100	-1.53002700	-1.60355600
H	-1.56210600	-2.45578900	-0.26182100
C	-0.87011600	-0.04441500	1.91946400
H	-1.82402100	-0.08500800	2.45907500
H	-0.28368700	-0.92316200	2.21154500
H	-0.32748100	0.84331200	2.26328500
C	-2.10837400	1.56286700	-0.43677200
H	-1.58893900	2.47409000	-0.11720500
H	-2.24970000	1.62375200	-1.52277200
H	-3.10312200	1.57318900	0.02556900

TS-16

H	2.25130800	-0.33869600	-0.81422700
Si	5.01258000	-0.80985000	0.03253100
C	5.45900700	-1.76399600	-1.54674800
H	6.37530800	-2.34700800	-1.38844000
H	5.63993800	-1.08683500	-2.38944500
H	4.66923200	-2.46293600	-1.84332400
C	4.47525800	-2.07340100	1.35277000
H	5.27451200	-2.79740500	1.55525700
H	3.59408000	-2.63822000	1.02016100
H	4.22309600	-1.58804600	2.30379500
C	6.59525100	0.05990100	0.62957500
H	6.41536700	0.59643800	1.56856500
H	6.92973400	0.79858300	-0.10917000
H	7.42016300	-0.64542600	0.79358800
O	1.26973900	-0.69757900	-1.18147200
C	1.12901300	-0.62089100	-2.60640400
C	0.09373300	-1.68707100	-3.01012800
H	-0.80587500	-1.63569800	-2.38404100
H	0.51247000	-2.69203900	-2.87510800
H	-0.19752600	-1.58968500	-4.06524200
C	0.65128300	0.79228100	-2.99971300
H	1.41506900	1.52765500	-2.72252200
H	-0.27487700	1.06916600	-2.47765500
H	0.47657400	0.87799300	-4.08061400
C	2.45439400	-0.91430400	-3.32415500
H	3.21016000	-0.17343800	-3.05272900
H	2.31502100	-0.88906900	-4.41248600
H	2.82383000	-1.90752400	-3.05136900
K	0.29557200	1.58627200	0.34307600
C	3.48376400	2.63710100	-0.75115900
C	3.21950000	2.56601300	0.60880600
C	3.27290400	1.21875500	0.99117800
C	3.57793900	0.39915200	-0.18217400
H	3.16866700	0.83655900	1.99989700
O	-0.63358100	-0.06736300	2.22940900
K	-0.23554500	-2.03809400	0.58179000
C	-0.30585400	-0.06782100	3.57925200
C	0.38023900	1.26274200	3.98190900
H	0.63829400	1.30739600	5.04846100
H	1.30371700	1.39944000	3.40585100

H	-0.28811200	2.10638400	3.76059300
C	-1.57657900	-0.23624100	4.45783200
H	-2.10449000	-1.16116100	4.18494500
H	-1.35365100	-0.28301300	5.53189000
H	-2.26021700	0.61303700	4.30632400
C	0.66010900	-1.23629200	3.90937900
H	1.56422800	-1.15910300	3.29219200
H	0.97038500	-1.25599000	4.96253000
H	0.17421700	-2.19994500	3.69328100
O	-2.31715600	1.91058100	-0.51299100
O	-2.77148000	-1.70325900	-0.35954100
K	-3.05314300	0.26961300	1.43185600
K	-2.84851200	0.09010000	-2.21727400
C	-3.60317600	-2.81491600	-0.40186200
C	-2.80451100	-4.12203600	-0.14928400
H	-2.35566600	-4.10306900	0.85466700
H	-3.42643200	-5.02461600	-0.20819200
H	-2.00099600	-4.22055900	-0.89186300
C	-4.29345700	-2.94220500	-1.78783900
H	-4.94374500	-3.82278300	-1.86843100
H	-4.92179600	-2.05893400	-1.98069200
H	-3.53550800	-3.01370600	-2.58011900
C	-4.71335900	-2.71603900	0.67832700
H	-4.26017200	-2.65053600	1.67729300
H	-5.31923800	-1.81342900	0.51250100
H	-5.39504700	-3.57673800	0.67872500
C	-2.78891600	3.21107200	-0.64589000
C	-3.44523400	3.42481100	-2.03785100
H	-4.30321000	2.74564500	-2.16134100
H	-3.81854700	4.44611000	-2.18766000
H	-2.71559500	3.21823900	-2.83333300
C	-3.85575300	3.52210100	0.43788200
H	-3.41771300	3.40540000	1.43902700
H	-4.25809100	4.54129600	0.36905800
H	-4.70087300	2.82433600	0.34488700
C	-1.63939100	4.24198900	-0.49930500
H	-1.97480100	5.27897400	-0.63107300
H	-1.19035300	4.16965700	0.50149700
H	-0.85799300	4.04512400	-1.24547500
H	3.01972600	3.42038100	1.24893600
H	3.67417300	3.47739000	-1.40467300
O	3.81236400	1.39189100	-1.25116200

TS-17

H	2.46727900	0.76767500	-0.11636900
Si	5.29359600	0.43394700	-0.00112800
C	5.67823900	1.42585800	1.57791100
H	6.72475300	1.75643800	1.57319400
H	5.54228100	0.79662700	2.46679300
H	5.05436000	2.31669100	1.70861600
C	5.58916500	1.51040500	-1.54184000
H	6.62680600	1.86601000	-1.57607300
H	4.93422000	2.38685500	-1.57552600
H	5.41504800	0.93082400	-2.45748100
C	6.56863800	-0.97804200	-0.05508800
H	6.45924200	-1.57753800	-0.96649400
H	6.43844700	-1.65512600	0.79783400
H	7.59747600	-0.59677700	-0.02530400
O	1.43502200	1.37511300	-0.29228700
C	1.42664200	2.65294800	0.32622100
C	0.20142200	3.43877300	-0.18452300
H	-0.72802300	2.86094600	-0.11694200
H	0.33378900	3.70045800	-1.24321600

H	0.06885900	4.38113800	0.36399700
C	1.35850500	2.49150100	1.86076000
H	2.23093700	1.93825700	2.22247100
H	0.47567500	1.90451900	2.15148800
H	1.32155600	3.45783400	2.38083200
C	2.68051800	3.46862300	-0.04353200
H	3.58666800	2.99476500	0.33619400
H	2.63062000	4.48461400	0.36876600
H	2.76716700	3.54457700	-1.13327200
K	0.32231100	-1.33385900	0.77907700
C	2.94643100	-2.43119000	-0.57008900
C	3.27297600	-1.22201100	-1.06645900
C	3.53414800	-0.26596900	0.03975100
H	3.35326600	-0.99696200	-2.12484800
O	-1.09612900	-1.71414000	-1.47813900
K	-0.52909700	0.75329400	-2.03633800
C	-1.03651800	-2.76367800	-2.38596400
C	-0.59937400	-4.07520400	-1.68453700
H	-0.56404500	-4.93627500	-2.36546500
H	0.39761700	-3.95232300	-1.24458400
H	-1.29886400	-4.31334100	-0.87176600
C	-2.42425600	-3.00898500	-3.04020100
H	-2.78758700	-2.08370600	-3.50805900
H	-2.40448800	-3.79285600	-3.80897900
H	-3.15821100	-3.32138800	-2.28139000
C	-0.02283400	-2.45338500	-3.51949900
H	0.95855400	-2.22941600	-3.08444400
H	0.09586400	-3.28183300	-4.23055200
H	-0.35393700	-1.57540200	-4.09552900
O	-2.03206100	-0.75537000	2.05446400
O	-2.83757300	1.45153100	-0.71458900
K	-3.27613500	-1.14356200	-0.24247900
K	-2.29368500	1.75799200	1.78690400
C	-3.77132900	2.23710700	-1.37796600
C	-3.20310400	2.76944500	-2.72107100
H	-2.94724900	1.92803400	-3.38135100
H	-3.91279100	3.40573100	-3.26557900
H	-2.29607700	3.36139300	-2.53898100
C	-4.18085200	3.46302900	-0.51597400
H	-4.90583800	4.11917300	-1.01480900
H	-4.64323400	3.12649300	0.42466200
H	-3.29519900	4.06619300	-0.27459900
C	-5.05674800	1.42499800	-1.69275200
H	-4.81285200	0.56431800	-2.33124300
H	-5.50352700	1.05102500	-0.76002100
H	-5.82299700	2.01499800	-2.21263500
C	-2.34849700	-1.41861100	3.23407800
C	-2.70756200	-0.40805400	4.35838000
H	-3.57877900	0.19627700	4.06154000
H	-2.95856300	-0.89149100	5.31140700
H	-1.85862300	0.26558700	4.54365500
C	-3.56881500	-2.35462400	3.02480000
H	-3.33909000	-3.09956800	2.25027400
H	-3.85713600	-2.89923200	3.93349800
H	-4.44060300	-1.76962700	2.69683300
C	-1.15844600	-2.28015000	3.72876100
H	-1.37201200	-2.80508400	4.66904900
H	-0.90491300	-3.04161700	2.97820300
H	-0.27521400	-1.64798800	3.89133600
H	2.69821000	-3.37179500	-1.04313400
C	3.22669900	-1.09962700	1.22295300
H	3.76522400	-1.08825700	2.16861000
O	2.94209200	-2.44682000	0.81359300

C-20

C	2.71776200	-0.72639700	0.00013600
C	2.88334200	0.62484900	0.00019900
C	1.56289400	1.17828200	-0.00004200
C	0.67363500	0.13386100	-0.00022500
H	1.30381300	2.22883700	-0.00012400
Si	-1.20128900	0.00625800	-0.00000200
C	-1.76539700	-0.92939200	-1.54413000
H	-1.31276000	-1.92679000	-1.58701400
H	-2.85501700	-1.05661800	-1.55534900
H	-1.48028000	-0.39608500	-2.45836300
C	-1.88689900	1.76901900	-0.00555800
H	-2.98351600	1.75382300	-0.00396800
H	-1.56409400	2.33190600	0.87799400
H	-1.56647400	2.32513500	-0.89423700
C	-1.76614000	-0.91974000	1.54970200
H	-1.48031700	-0.38133500	2.46071900
H	-2.85590300	-1.04570100	1.56182500
H	-1.31460000	-1.91737200	1.59840600
H	3.82308500	1.15977100	0.00034700
H	3.40536800	-1.55944500	0.00021500
O	1.39794300	-1.04833000	-0.00011500

C-21

Si	-1.21701500	-0.00489100	-0.00004600
C	-1.82519700	1.78835800	-0.00083300
H	-2.92140200	1.82290500	-0.00109600
H	-1.48064800	2.33472400	0.88523600
H	-1.48022800	2.33423200	-0.88703700
C	-1.85438900	-0.89569300	-1.54507900
H	-2.95100700	-0.92503700	-1.56081300
H	-1.51987400	-0.39168200	-2.45933500
H	-1.49603000	-1.93120600	-1.58964400
C	-1.85448500	-0.89398700	1.54594000
H	-1.49698100	-1.92975800	1.59129200
H	-1.51927900	-0.38944700	2.45965100
H	-2.95112600	-0.92240300	1.56204800
C	2.82709500	-0.65352500	0.00013400
C	1.56222200	-1.14784800	0.00012300
C	0.65871300	-0.01437000	-0.00006400
H	3.80837200	-1.10375800	0.00023900
H	1.29026000	-2.19525100	0.00023800
O	2.80369500	0.71188300	-0.00003600
C	1.48904500	1.07250700	-0.00014000
H	1.30856200	2.13744900	-0.00032800

C-22

C	-0.01190200	-1.24340800	-0.00000100
C	-1.27302600	-0.71463500	-0.00000900
C	-1.27239500	0.71534800	0.00000700
C	-0.01079000	1.24310900	0.00003100
H	-2.17179700	1.32175600	0.00001300
H	-2.17315100	-1.31999100	-0.00001800
H	0.28061500	-2.28473500	-0.00000500
S	1.19948300	-0.00026300	-0.00001400
H	0.28128500	2.28469900	0.00005500

TS-18

C	0.90627600	0.07786600	-1.11060000
C	1.36511100	1.31445100	-0.65314200
C	2.31204500	1.20428200	0.39695600
C	2.65653900	-0.09365100	0.68310500

H	2.73034500	2.05643400	0.92294800
H	0.99949900	2.25739700	-1.04442500
H	0.45591700	-0.11437300	-2.07416300
S	1.82782500	-1.22109700	-0.35405100
H	3.33159000	-0.45530000	1.44688900
Si	-1.59798800	-0.03424200	0.01287300
C	-2.90837200	-1.31992600	-0.50571500
H	-3.81278000	-1.23459200	0.11395800
H	-3.20877800	-1.18638700	-1.55129300
H	-2.52729400	-2.34159000	-0.39567400
C	-1.13321500	-0.27990800	1.83648000
H	-1.99036300	-0.07902100	2.49383200
H	-0.79930600	-1.30620400	2.02452400
H	-0.31908300	0.39246200	2.12776100
C	-2.27725700	1.72316500	-0.25612900
H	-1.52300400	2.47840100	-0.00823900
H	-2.58297300	1.88241900	-1.29677400
H	-3.15390000	1.90961800	0.37951600

TS-19

C	-1.41695200	1.02744600	-0.71180500
C	-0.67150600	-0.03863900	-1.22670100
C	-1.21899300	-1.31084700	-0.78483900
C	-2.21864600	-1.18180700	0.12311700
H	-0.83744800	-2.26977800	-1.12015000
H	-0.12147700	0.05880000	-2.15701300
H	-1.30224100	2.08117900	-0.92436100
S	-2.60251100	0.49539700	0.45021700
H	-2.75748200	-1.96609200	0.63841600
Si	1.59247900	-0.00658700	0.04411400
C	2.23832700	1.73670000	-0.36025300
H	3.08669300	2.00408800	0.28436300
H	2.57773600	1.80956000	-1.40030900
H	1.45842200	2.49168100	-0.20856000
C	1.09296000	-0.10581700	1.87191200
H	1.94575700	0.12386100	2.52541600
H	0.29232100	0.60550600	2.10076700
H	0.73177400	-1.10670800	2.13245000
C	2.95357000	-1.29188500	-0.32642800
H	2.60764700	-2.31075300	-0.11753800
H	3.26629400	-1.25441300	-1.37636600
H	3.84490100	-1.11196800	0.29181300

C-23

C	0.37579600	0.12393000	-0.80768300
C	1.12115500	1.39460800	-0.52260000
C	2.33078300	1.23343400	0.12555300
C	2.69737400	-0.08918800	0.36713100
H	2.96265100	2.06660500	0.42095700
H	0.70658600	2.35532900	-0.80995800
H	0.20705500	-0.01715000	-1.88691900
S	1.51527000	-1.24008900	-0.23491900
H	3.59341900	-0.44504000	0.85794300
Si	-1.34299600	0.01548700	0.07059800
C	-2.12584100	-1.65885900	-0.33597800
H	-3.11823300	-1.74690600	0.12301400
H	-2.24948800	-1.79450700	-1.41730200
H	-1.51363500	-2.48755200	0.03789200
C	-1.12063100	0.21955700	1.93330700
H	-2.08667400	0.17491200	2.45067200
H	-0.48263700	-0.57165600	2.34167300
H	-0.65422600	1.18143000	2.17348300
C	-2.42038500	1.41027000	-0.62749800

H	-1.99981100	2.39779700	-0.40425100
H	-2.52927000	1.33146900	-1.71606400
H	-3.42761900	1.37735700	-0.19419600

C-24

C	1.15196400	-1.03119400	-0.53579900
C	0.25221800	0.12163000	-0.86114900
C	1.00704100	1.36037200	-0.46181100
C	2.21187200	1.15507600	0.08878800
H	0.59089400	2.35439400	-0.60017700
H	-0.00972000	0.15314100	-1.93778000
H	1.02867200	-2.04347000	-0.89640200
S	2.67660500	-0.55283300	0.18080800
H	2.89829400	1.90549100	0.46264100
Si	-1.44633700	-0.03925500	0.06731100
C	-2.27416200	-1.64681500	-0.49632000
H	-3.25433600	-1.76928000	-0.01940800
H	-2.43274000	-1.65976700	-1.58165700
H	-1.66862900	-2.52252300	-0.23610600
C	-1.15362000	-0.06240700	1.93291500
H	-2.09811400	-0.17620600	2.47876900
H	-0.49844200	-0.89364900	2.21545200
H	-0.67911000	0.86446000	2.27459700
C	-2.54627200	1.43104600	-0.41093300
H	-2.11424100	2.38554100	-0.08750800
H	-2.69750900	1.48439200	-1.49607700
H	-3.53622000	1.34612200	0.05423800

TS-20

H	2.27395300	-0.33777200	-0.74214500
Si	4.88125300	-1.03816400	0.02548700
C	5.70771600	-1.37107300	-1.65037400
H	6.57087900	-2.03546900	-1.51654000
H	6.07739400	-0.43894400	-2.09454600
H	5.03541700	-1.84244300	-2.37378000
C	4.08482300	-2.65055000	0.65961100
H	4.83061200	-3.44414500	0.79470800
H	3.32914300	-3.01544300	-0.04778100
H	3.59372300	-2.49456800	1.62963200
C	6.25858700	-0.54303300	1.23703000
H	5.86090600	-0.37394400	2.24445700
H	6.73569000	0.39038000	0.91454200
H	7.03815600	-1.31271000	1.30484600
O	1.23479800	-0.69837800	-1.10911900
C	1.08006200	-0.76630100	-2.52624500
C	0.05260000	-1.87645700	-2.82733600
H	-0.85629600	-1.76909600	-2.22208300
H	0.47749900	-2.85854300	-2.58360800
H	-0.22680600	-1.89661000	-3.88965800
C	0.59026700	0.59778200	-3.05906100
H	1.35828200	1.35924000	-2.88000600
H	-0.31960000	0.92869000	-2.54016300
H	0.38816000	0.57083000	-4.13834700
C	2.39941300	-1.12777300	-3.22756200
H	3.15553300	-0.35602000	-3.06206900
H	2.24956300	-1.23045800	-4.30971400
H	2.78384100	-2.07937500	-2.84552400
K	0.23625800	1.60979900	0.31125900
C	3.34750500	2.88511600	0.14648800
C	3.05417900	2.20277300	1.33252700
C	3.13649100	0.81612400	1.24089900
C	3.51896800	0.26912100	-0.06766100
H	2.95050200	0.16306100	2.09048600

O	-0.79499000	0.04991800	2.24230300
K	-0.31408000	-1.97228000	0.67246200
C	-0.57077300	0.02853500	3.61251600
C	0.18810000	1.29921800	4.06991100
H	0.37155700	1.32373100	5.15251900
H	1.15584300	1.35951400	3.55922600
H	-0.39294500	2.19296000	3.80442500
C	-1.91201500	-0.03495900	4.39645200
H	-2.48822600	-0.92160600	4.09396200
H	-1.77182900	-0.08618400	5.48424200
H	-2.51473300	0.86261200	4.19076700
C	0.26980900	-1.21376100	4.01338000
H	1.22355600	-1.20844800	3.46951100
H	0.49533700	-1.25498100	5.08717900
H	-0.27256500	-2.13667800	3.75713600
O	-2.35261200	1.89475800	-0.67222800
O	-2.84294300	-1.70184800	-0.34279300
K	-3.17330800	0.36505500	1.32632900
K	-2.87263300	-0.00783300	-2.29056100
C	-3.66927700	-2.81823800	-0.33838300
C	-2.87954000	-4.09721400	0.04876400
H	-2.46811100	-3.99328500	1.06326700
H	-3.49757900	-5.00426500	0.04059300
H	-2.04928600	-4.25257800	-0.65365900
C	-4.29551900	-3.05298200	-1.74057500
H	-4.93619100	-3.94313200	-1.78524200
H	-4.92016600	-2.19224200	-2.02550400
H	-3.50209100	-3.17384900	-2.49066400
C	-4.82792900	-2.64433000	0.67992200
H	-4.42175400	-2.50505000	1.69146000
H	-5.42536600	-1.75799800	0.42117700
H	-5.50904300	-3.50491300	0.71165100
C	-2.81092800	3.18990500	-0.88315200
C	-3.41540100	3.34104800	-2.30655300
H	-4.27302300	2.66111200	-2.42917000
H	-3.77687400	4.35588200	-2.51720400
H	-2.65930700	3.09397700	-3.06478200
C	-3.91449300	3.55736100	0.14505500
H	-3.51372100	3.48863800	1.16604100
H	-4.30891100	4.57339300	0.01228300
H	-4.75978800	2.85918200	0.05573200
C	-1.66116100	4.22110400	-0.74318300
H	-1.98546600	5.25248100	-0.93348400
H	-1.24793300	4.19224800	0.27501000
H	-0.85553700	3.98732300	-1.45182800
H	2.77759100	2.72651600	2.24614800
H	3.46692300	3.95244800	0.01043000
S	3.90150700	1.75854100	-1.10132300
TS-21			
H	2.32456100	-0.41412500	-0.74440500
Si	4.77188800	-1.16803600	0.03975700
C	5.67742100	-1.65962000	-1.55468800
H	6.42760800	-2.43061800	-1.33779800
H	6.20817500	-0.80016300	-1.98176800
H	5.00783300	-2.05406800	-2.32481200
C	3.83001200	-2.68304600	0.71550100
H	4.50537200	-3.51648200	0.94649500
H	3.09204600	-3.03352600	-0.01649800
H	3.29503500	-2.42937800	1.64138800
C	6.11346000	-0.70667900	1.30775000
H	5.68147300	-0.47766200	2.28924000
H	6.66583500	0.18259000	0.98063400

H	6.83850500	-1.51990600	1.44274400
O	1.22175100	-0.82783700	-1.08749300
C	1.05067300	-0.99978800	-2.48873200
C	-0.01132700	-2.09864500	-2.70839700
H	-0.91223400	-1.92307900	-2.10700000
H	0.38649700	-3.07345800	-2.39784500
H	-0.29951000	-2.18627900	-3.76527000
C	0.60026000	0.33337500	-3.12772200
H	1.38602600	1.08522300	-2.98763800
H	-0.31108300	0.72153100	-2.65122300
H	0.41171900	0.23593300	-4.20542100
C	2.35297100	-1.45098200	-3.17328600
H	3.12700800	-0.68648700	-3.07019000
H	2.19197700	-1.63379100	-4.24338000
H	2.71636300	-2.37982100	-2.72047400
K	0.25443300	1.60001000	0.11020300
C	3.16877400	2.25570700	1.04437300
C	3.16669400	0.89888600	1.02822900
C	3.53336200	0.24133800	-0.23492100
H	2.90167000	0.33263700	1.92027500
O	-0.68253300	0.19079300	2.20173700
K	-0.30495600	-1.96393300	0.77510400
C	-0.42512700	0.26475500	3.56412900
C	0.35231500	1.55846400	3.91481000
H	0.55903100	1.65619400	4.98902900
H	1.30963800	1.57767100	3.38159300
H	-0.22825900	2.43634400	3.60031900
C	-1.74680100	0.26909600	4.38409600
H	-2.33834600	-0.62993900	4.15706600
H	-1.57929700	0.28922300	5.46900500
H	-2.34655200	1.15735600	4.13421500
C	0.41501500	-0.95390200	4.03338000
H	1.35135200	-1.00351700	3.46213400
H	0.67374900	-0.91620000	5.09979000
H	-0.14351900	-1.88723700	3.86514900
O	-2.35222200	1.86694700	-0.75069200
O	-2.85728200	-1.70237800	-0.19257300
K	-3.10421800	0.45748900	1.35742700
K	-2.89368500	-0.13137700	-2.24221900
C	-3.70142600	-2.80211500	-0.10910500
C	-2.92107600	-4.07511000	0.31479100
H	-2.47461000	-3.92918300	1.30915000
H	-3.55439900	-4.96980000	0.37171900
H	-2.11703700	-4.27971700	-0.40508900
C	-4.37571300	-3.09248100	-1.47836800
H	-5.03526300	-3.96966200	-1.45826300
H	-4.99155600	-2.23367800	-1.78722400
H	-3.60915200	-3.26853700	-2.24545200
C	-4.82496700	-2.55988500	0.93452800
H	-4.38523200	-2.37849000	1.92519400
H	-5.41758100	-1.67775300	0.65165900
H	-5.51683500	-3.40713900	1.02882500
C	-2.82650200	3.14635300	-1.01657600
C	-3.44215000	3.22485200	-2.44064800
H	-4.29575200	2.53405400	-2.52431500
H	-3.81205300	4.22593200	-2.69742400
H	-2.68953000	2.94565500	-3.19099400
C	-3.92719900	3.54782900	0.00214500
H	-3.51726300	3.53682500	1.02186200
H	-4.33767900	4.55021100	-0.17726300
H	-4.76243800	2.83369300	-0.04493700
C	-1.68768500	4.19494200	-0.93032200
H	-2.02735600	5.21543100	-1.14993300

H	-1.25910600	4.20420100	0.08186100
H	-0.88999100	3.94849500	-1.64375900
H	2.94219600	2.90972400	1.87918300
S	3.66317500	2.94932500	-0.51590800
C	3.82868500	1.30961100	-1.21431700
H	4.51512000	1.21456400	-2.04975900

C-25

C	2.95137300	-0.16752000	0.00002100
C	2.61567500	1.15837000	0.00001900
C	1.20321000	1.36342200	0.00000000
C	0.45554700	0.20485500	-0.00001400
H	0.75066400	2.35024700	-0.00001600
Si	-1.41944000	0.02732200	0.00000500
C	-1.97082000	-0.91596800	-1.54526200
H	-1.52495800	-1.91690400	-1.58590100
H	-3.06101100	-1.03793100	-1.56429800
H	-1.67638500	-0.38637900	-2.45865200
C	-2.16568000	1.76586000	-0.00086000
H	-3.26109000	1.71010900	-0.00025200
H	-1.86448500	2.33720300	0.88479500
H	-1.86537300	2.33589100	-0.88766000
C	-1.97097900	-0.91450400	1.54610900
H	-1.67673000	-0.38399100	2.45902300
H	-3.06116200	-1.03654500	1.56509900
H	-1.52502300	-1.91535400	1.58778900
H	3.34509800	1.96164600	0.00002700
H	3.93902200	-0.60987700	0.00002400
S	1.54022800	-1.17235600	-0.00000800

C-26

Si	1.53858000	0.03017500	0.00001500
C	2.22009500	-0.82777100	1.54542600
H	3.31685700	-0.80342500	1.55949700
H	1.86276900	-0.34030000	2.46000100
H	1.91289700	-1.87955000	1.59096800
C	2.21965700	-0.82825100	-1.54533400
H	3.31641700	-0.80411500	-1.55975000
H	1.91225200	-1.87998800	-1.59050700
H	1.86213800	-0.34096700	-2.45993300
C	2.05343400	1.85161900	-0.00032300
H	1.68128600	2.37940100	-0.88647000
H	1.68179900	2.37965700	0.88588200
H	3.14646900	1.94220200	-0.00065700
C	-2.45693100	-1.12559100	0.00004100
C	-1.10375300	-1.31008000	0.00008800
C	-0.34360700	-0.08461400	0.00010800
H	-3.23730700	-1.87515600	0.00001300
H	-0.65214300	-2.29774800	0.00010600
C	-1.18496100	1.00253400	0.00006000
H	-0.91819400	2.05150300	0.00007200
S	-2.86556000	0.56118500	0.00001000

TS-4

C	2.33045100	-0.49880100	1.76744400
H	1.80032700	-1.41849000	2.04164200
H	3.31693600	-0.51976900	2.25066500
H	1.75619900	0.33392300	2.19219000
C	1.80997600	1.23968000	-0.98868800
H	1.43405400	1.95462800	-0.24575000
H	2.59349700	1.73814200	-1.57564100
H	0.96788300	1.01814200	-1.65269100
C	2.21777100	-1.98245100	-1.12607800

H	1.49972200	-1.84294000	-1.94305400
H	3.17043800	-2.32194500	-1.54920000
H	1.81923800	-2.77471500	-0.48067700
Si	2.42437200	-0.36148600	-0.14347600
C	4.69481300	1.85482600	0.77932400
C	5.18562200	0.63004600	-0.02246400
H	3.97611300	2.44249500	0.20044300
H	4.21209000	1.54906300	1.71269500
H	5.53882700	2.50900600	1.03534800
C	6.20633100	-0.15683700	0.82708000
C	5.86869900	1.11618600	-1.31797800
H	6.55030800	-1.03466200	0.26864900
H	7.08010700	0.45405000	1.09269300
H	5.73727500	-0.50973800	1.75245600
H	6.73228100	1.76333500	-1.11152600
H	6.20999200	0.25322300	-1.90068200
H	5.15513200	1.67616300	-1.93279500
O	4.16222100	-0.26408500	-0.39559900
H	0.45801200	-0.58119200	0.10154000
C	-3.37401700	2.58568400	1.23694300
C	-2.95307200	1.46581000	0.52650900
C	-2.98851700	1.41654700	-0.91094200
C	-3.51834800	2.53321300	-1.60622400
C	-3.96341200	3.64513200	-0.88386500
C	-3.89268600	3.68370300	0.51332700
H	-3.31414900	2.61920900	2.32215100
H	-3.55990200	2.52818600	-2.69372500
H	-4.36473800	4.50331000	-1.42190600
H	-4.23444500	4.56559000	1.05128900
C	-2.42989500	0.18817200	-1.29695300
C	-1.97802500	-0.55779000	-0.12463500
H	-0.57702700	-0.59575700	-0.03274400
N	-2.44303500	0.26836500	0.99548200
H	-2.29825800	-0.15336400	-2.31733500
C	-1.87520700	0.17063300	2.32065000
H	-1.02545200	0.85763700	2.46304600
H	-2.63212100	0.40292200	3.08243500
H	-1.51819500	-0.84593000	2.49243800
Si	-2.45179700	-2.39129200	-0.11018900
C	-4.32892200	-2.66885900	0.06390800
H	-4.70062100	-2.23233100	0.99893600
H	-4.86731900	-2.18299100	-0.75821400
H	-4.59120000	-3.73556300	0.06158100
C	-1.58975700	-3.35422200	1.29133900
H	-1.69709600	-4.43748800	1.14555100
H	-0.51827900	-3.12254600	1.31505000
H	-2.00671600	-3.11625400	2.27782200
C	-1.86863900	-3.15106300	-1.75181400
H	-0.78821200	-3.01581300	-1.87876800
H	-2.07897600	-4.22810100	-1.78823700
H	-2.36729600	-2.68407600	-2.60924200
TS-5			
H	0.64634900	0.64751600	-0.01343900
Si	2.68970900	2.10709700	-0.12052400
C	2.04439900	3.36862100	1.14817000
H	2.40743500	4.38116700	0.92706400
H	2.36874900	3.11562400	2.16531000
H	0.94858100	3.39248300	1.14617500
C	2.14175100	2.68347100	-1.84798500
H	2.40526300	3.73488600	-2.02429100
H	1.05527500	2.58141700	-1.95258400
H	2.61069700	2.08782400	-2.64037800

C	4.59710100	2.14532900	-0.05898900
H	5.02429300	1.45026700	-0.79211000
H	4.95802800	1.83937800	0.93080900
H	4.99842800	3.14635400	-0.26890700
C	2.72068800	-1.82914900	0.36491600
C	2.37305500	-0.76603000	-0.51693700
C	1.98023500	0.41878300	0.28544500
C	2.61912800	-2.23056900	2.81683900
H	3.40037700	-2.99683400	2.74650500
H	1.64456500	-2.73513300	2.93379800
H	2.80506400	-1.63890600	3.71997900
N	2.66300900	-1.36287200	1.66827900
C	2.11171700	-0.05188800	1.68203700
H	2.38250500	0.57000700	2.53537300
C	2.37160300	-1.01727500	-1.89091100
C	3.03924200	-3.10613700	-0.10352700
C	3.04345700	-3.32213000	-1.49242600
C	2.71642700	-2.29327000	-2.37400500
H	2.70924300	-2.48058800	-3.44603400
H	3.29258700	-4.30961100	-1.87678800
H	2.08280100	-0.23522600	-2.58833100
H	3.27754800	-3.91636700	0.58142000
C	-1.68018900	-0.95967400	1.00115700
H	-0.82052100	-0.70183100	1.63086000
H	-2.46601100	-1.39107000	1.63631300
H	-1.33291300	-1.73959000	0.31080300
C	-2.21678500	0.56974100	-1.88953700
H	-1.64203900	-0.28978600	-2.25583400
H	-3.20928400	0.55189400	-2.36062700
H	-1.69258700	1.46707500	-2.24001400
C	-2.08251100	2.27363100	0.89390200
H	-1.71052900	3.02247900	0.18319800
H	-3.03259200	2.62787500	1.31046700
H	-1.34453800	2.20480900	1.70212400
Si	-2.26971500	0.58113500	0.03033000
C	-4.56538000	-1.69624300	-0.70064300
C	-5.04545200	-0.40629700	0.00104800
H	-4.07865600	-1.47011900	-1.65429900
H	-3.85125800	-2.24101100	-0.07590100
H	-5.41463400	-2.36216700	-0.90479600
C	-5.73644800	-0.78535500	1.32887900
C	-6.06246900	0.31629400	-0.90960800
H	-6.07374300	0.12334000	1.84033300
H	-6.60368800	-1.44191900	1.17146900
H	-5.02773300	-1.29859400	1.98850300
H	-6.93818600	-0.30972900	-1.13125900
H	-6.40457800	1.23545600	-0.42055300
H	-5.58887100	0.59654900	-1.85716100
O	-4.01837700	0.50492300	0.30495500
H	-0.37681000	0.77643000	-0.23903100

TS-22

C	1.70979000	-0.87048100	1.66101000
H	1.01961600	-1.71768700	1.74932700
H	2.66731500	-1.16616800	2.11382300
H	1.28407900	-0.05496000	2.25869200
C	1.56021600	1.46490100	-0.65006700
H	1.28301500	2.05633800	0.23201400
H	2.43853700	1.93457500	-1.11464600
H	0.71583700	1.54160900	-1.34308400
C	1.30032200	-1.66210200	-1.46165000
H	0.57012800	-1.22735800	-2.15326500
H	2.14861100	-2.05244000	-2.03731100

H	0.80461000	-2.50234200	-0.95974800
Si	1.85224900	-0.36372600	-0.18228400
C	4.52435800	1.10207500	1.09078800
C	4.75491000	0.00007300	0.03380000
H	3.94900600	1.93421800	0.67390800
H	3.98149300	0.71168400	1.95709500
H	5.48523900	1.49832400	1.44539500
C	5.58171800	-1.14096800	0.66383700
C	5.53548200	0.59856800	-1.15527200
H	5.74162600	-1.93205500	-0.07738100
H	6.56055200	-0.79216300	1.02102800
H	5.04010100	-1.57790900	1.51033000
H	6.51287200	0.99623400	-0.84881100
H	5.69503900	-0.17270900	-1.91712800
H	4.95892100	1.40983400	-1.61371600
O	3.57132700	-0.56471900	-0.48214500
H	-0.16826100	-0.22658900	0.10475600
C	-2.72036200	2.82465400	0.00406500
C	-2.66811600	2.54475900	-1.35222500
C	-2.60367700	1.15800200	-1.52901800
C	-2.53838100	0.50631400	-0.21668900
H	-1.10252800	0.02216100	-0.00395800
N	-2.77623400	1.61482200	0.72968500
H	-2.50796800	0.63723100	-2.47524400
C	-2.13177000	1.57318400	2.02823400
H	-1.03062000	1.62079300	1.96451500
H	-2.47766100	2.42183300	2.63402300
H	-2.39813200	0.65179600	2.55576400
Si	-3.52965300	-1.06728200	0.01584200
C	-5.42525600	-0.82207100	-0.02659800
H	-5.73709100	-0.12124600	0.75790100
H	-5.73271100	-0.39055100	-0.98706400
H	-5.97871000	-1.76055400	0.11855600
C	-3.12603400	-1.94845900	1.66046600
H	-3.56617200	-2.95462000	1.68978800
H	-2.04173300	-2.04955600	1.78783800
H	-3.51349300	-1.39829200	2.52724800
C	-3.06167200	-2.26514400	-1.38839000
H	-1.98036900	-2.44666800	-1.39714400
H	-3.56774400	-3.23391800	-1.28125800
H	-3.33500200	-1.85301800	-2.36745800
H	-2.68529600	3.29238900	-2.14046500
H	-2.83560300	3.77006700	0.52149100

TS-23

H	-1.12538800	-0.40814700	-0.24628300
Si	-3.47389800	-1.15775100	0.16015100
C	-2.95323600	-1.96631000	1.80264300
H	-3.54058000	-2.86766400	2.02306700
H	-3.07917900	-1.27266200	2.64377800
H	-1.89445100	-2.24802500	1.76443000
C	-3.26607300	-2.44842900	-1.22550400
H	-3.83846400	-3.36366900	-1.02386400
H	-2.20926500	-2.72232600	-1.32680900
H	-3.60114900	-2.05528000	-2.19408200
C	-5.33819800	-0.74733700	0.29807600
H	-5.71839800	-0.33369300	-0.64448600
H	-5.50818800	0.00747700	1.07600900
H	-5.94380900	-1.63021700	0.54713000
C	-2.48895500	2.38090300	-1.22512500
C	-2.49529700	1.04727900	-1.45335100
C	-2.37157300	0.31129600	-0.17302500
C	-1.81038400	3.83839900	0.65216000

H	-2.12070800	4.71462700	0.06778800
H	-0.70747700	3.76088400	0.62081100
H	-2.10208500	4.00928300	1.69617500
N	-2.47163200	2.65211800	0.15280500
C	-2.27134100	1.40123000	0.81711600
H	-2.60197100	1.34551200	1.85435400
C	1.29873000	-0.04116800	1.52479500
H	0.81404900	-0.83195100	2.11286300
H	2.15610500	0.32285600	2.10785600
H	0.55904100	0.76310200	1.42885500
C	1.47492600	0.30419700	-1.75493400
H	0.88332400	1.19721000	-1.52175200
H	2.40978100	0.61388200	-2.24170300
H	0.88938400	-0.27049300	-2.48262600
C	1.60046000	-2.65581500	-0.41609600
H	1.04270600	-2.88687300	-1.33163900
H	2.58262000	-3.14166800	-0.46686400
H	1.03568800	-3.09259600	0.41689700
Si	1.75210200	-0.76315400	-0.18934700
C	4.07964100	1.60631200	0.10282700
C	4.54214000	0.13234500	0.13397900
H	3.67697200	1.87182900	-0.87951500
H	3.30229100	1.79472000	0.84911200
H	4.92300600	2.27721700	0.31547300
C	5.16280600	-0.17743100	1.51453900
C	5.61346500	-0.07602200	-0.95818200
H	5.48879600	-1.22341400	1.54303800
H	6.02771000	0.46504000	1.73180200
H	4.42009400	-0.03558600	2.30699000
H	6.48828400	0.57226800	-0.80929100
H	5.94645000	-1.12012100	-0.95354500
H	5.18702600	0.13621800	-1.94525200
O	3.52022700	-0.80262000	-0.11077400
H	-0.20061400	-0.84846800	-0.28783100
H	-2.55828900	0.58708400	-2.43448000
H	-2.50123100	3.20576200	-1.93061800
TS-24			
C	-1.53510000	-1.17321500	-1.43348800
H	-0.80840600	-1.98883700	-1.34247100
H	-2.47298900	-1.59687900	-1.82058100
H	-1.13401100	-0.47879100	-2.18162300
C	-1.46454600	1.58231200	0.37501700
H	-1.15124200	1.98982700	-0.59422800
H	-2.36231300	2.12435000	0.70427300
H	-0.64947300	1.80202700	1.07239100
C	-1.23710300	-1.32823800	1.79405400
H	-0.55910200	-0.75305400	2.43488900
H	-2.11329500	-1.62690300	2.38237900
H	-0.69684400	-2.23269900	1.48821700
Si	-1.73296800	-0.30626400	0.26402500
C	-4.34502000	0.84938500	-1.38406600
C	-4.62379600	0.00777100	-0.11946900
H	-3.75701500	1.74034100	-1.14416900
H	-3.79477400	0.26931200	-2.13127100
H	-5.28797500	1.17881600	-1.84040900
C	-5.45819800	-1.23036900	-0.51046900
C	-5.42025600	0.86188500	0.88956000
H	-5.65521400	-1.83765000	0.38016200
H	-6.41907800	-0.95348800	-0.96602600
H	-4.90227200	-1.84965300	-1.22342000
H	-6.38047800	1.20098800	0.47668000
H	-5.61606700	0.27582900	1.79457200

H	-4.83690100	1.74290700	1.17972700
O	-3.46504600	-0.45169600	0.53746200
H	0.27739600	-0.20873600	0.03039700
C	2.71768000	2.75130100	-0.75037800
C	2.75663300	2.86646500	0.62201400
C	2.74946100	1.57436100	1.16900000
C	2.61288100	0.61953500	0.07537900
H	1.21185300	0.06929100	0.06330600
H	2.71284800	1.31708100	2.22087800
Si	3.63686900	-0.94025500	-0.06655800
C	5.51714700	-0.65320900	-0.25755000
H	5.72191000	-0.05255800	-1.15237400
H	5.91298000	-0.10079400	0.60366800
H	6.08129800	-1.59246400	-0.34652600
C	3.05366700	-1.94404400	-1.57110200
H	3.59668400	-2.89279800	-1.67594600
H	1.98349600	-2.16615900	-1.48808700
H	3.19643900	-1.36813600	-2.49342800
C	3.35532300	-1.96753900	1.51145300
H	2.28648900	-2.16360100	1.65742700
H	3.87452400	-2.93411200	1.46749500
H	3.71849100	-1.43572500	2.40007400
H	2.77661500	3.80397800	1.16875000
H	2.70842500	3.47791700	-1.55107000
O	2.69138900	1.42585200	-1.13720100

TS-25

H	1.22062800	0.04442700	0.19179000
Si	3.53981700	-0.95918600	0.02487500
C	3.12352000	-1.94787500	-1.54608100
H	3.67512100	-2.89641900	-1.59185800
H	3.37203300	-1.37597100	-2.44935200
H	2.05186100	-2.17415200	-1.58541100
C	3.10826500	-2.03109000	1.53859700
H	3.61231500	-3.00634500	1.51109800
H	2.02658200	-2.20594000	1.57621900
H	3.39507200	-1.53687000	2.47579300
C	5.43066400	-0.67141200	0.02838100
H	5.74389000	-0.14204100	0.93697900
H	5.72674200	-0.05105600	-0.82688800
H	5.99728500	-1.61154900	-0.02633700
C	2.80009500	2.81069800	0.70233000
C	2.68064700	1.55994000	1.18364300
C	2.52801000	0.61390800	0.05112100
C	2.56277000	1.52558900	-1.10449800
H	3.02130800	1.33130200	-2.07288700
C	-1.33985000	1.47262800	-0.50538100
H	-0.41437600	1.57549800	-1.08298400
H	-2.16486100	1.92693500	-1.07163900
H	-1.19460900	2.05882200	0.41165300
C	-1.66029200	-0.91973300	1.75497700
H	-1.26666800	-0.12416600	2.39992400
H	-2.65170700	-1.21074900	2.12983500
H	-0.98878200	-1.77860200	1.87310700
C	-1.11089100	-1.65763800	-1.37668600
H	-0.64529900	-2.51760000	-0.87880000
H	-1.95385200	-2.01663400	-1.97891700
H	-0.35548700	-1.22556200	-2.04327400
Si	-1.65789100	-0.36521500	-0.08415200
C	-4.37523600	1.15551200	1.05919800
C	-4.57203100	0.05592400	-0.00792200
H	-3.86816000	0.76059500	1.94502600
H	-3.77740800	1.98252400	0.66473300

H	-5.34575400	1.55930000	1.37778300
C	-5.29751100	0.66546800	-1.22686800
C	-5.44100700	-1.07473900	0.58569900
H	-5.43474100	-0.10339800	-1.99560500
H	-6.28195100	1.07550500	-0.96114200
H	-4.69148900	1.46911400	-1.65993600
H	-6.43033900	-0.71411700	0.90053100
H	-5.57846300	-1.86366800	-0.16248000
H	-4.94270300	-1.51953900	1.45447000
O	-3.37681900	-0.51909400	-0.47592000
H	0.25843100	-0.30034700	0.28509300
H	2.63903100	1.29858100	2.23571700
H	2.87342100	3.77193500	1.19719300
O	2.80219900	2.85893600	-0.67015600

TS-26

C	-1.70850400	-1.17337600	-1.48000700
H	-0.99828900	-2.00572100	-1.41000800
H	-2.66455100	-1.57386500	-1.84503900
H	-1.31005500	-0.48394600	-2.23425500
C	-1.55821500	1.57470100	0.35346300
H	-1.27769600	1.99142400	-0.62194000
H	-2.44078400	2.11675200	0.72054500
H	-0.71841100	1.78100600	1.02530500
C	-1.35139400	-1.35525600	1.74641900
H	-0.62784900	-0.81402800	2.36663700
H	-2.22334100	-1.61265400	2.35914200
H	-0.86516100	-2.28506500	1.42503300
Si	-1.84343900	-0.31159900	0.22846400
C	-4.47528000	0.90492700	-1.35307600
C	-4.74051300	0.04790400	-0.09575200
H	-3.87645500	1.78773700	-1.11015400
H	-3.94086100	0.33116900	-2.11642300
H	-5.42239700	1.24798300	-1.79041800
C	-5.59657500	-1.17488000	-0.48940700
C	-5.51035400	0.89624700	0.93898400
H	-5.78340300	-1.79321700	0.39580700
H	-6.56278300	-0.88072900	-0.92235400
H	-5.06157500	-1.78968200	-1.22193900
H	-6.47410500	1.25112500	0.54807300
H	-5.69634400	0.29955000	1.83912700
H	-4.91282000	1.76706700	1.23117300
O	-3.57618100	-0.43256200	0.53379600
H	0.11495300	-0.25545900	-0.03986700
C	2.88184600	2.98567400	-0.14879600
C	2.78982300	2.58011800	1.17779500
C	2.61494700	1.21127700	1.36272200
C	2.45628700	0.41991900	0.13971200
H	1.09533900	0.00401200	0.03269600
H	2.51516600	0.75027800	2.34216400
Si	3.37927300	-1.20274200	-0.03166800
C	5.27628400	-1.01660200	-0.04286900
H	5.58803200	-0.36087500	-0.86451200
H	5.62706400	-0.55997300	0.89070900
H	5.78828700	-1.98133600	-0.16300300
C	2.86275300	-2.06321300	-1.64593600
H	3.31497800	-3.05939400	-1.74038300
H	1.77303600	-2.17596700	-1.68516800
H	3.16508200	-1.47485300	-2.52117500
C	2.89942700	-2.32233400	1.43059000
H	1.81135600	-2.44570400	1.48069400
H	3.35157100	-3.31915700	1.34234600
H	3.22772400	-1.89275600	2.38526900

H	2.84313600	3.28867100	2.00316300
H	2.96609100	3.99170500	-0.53844700
S	2.73372900	1.60790900	-1.24696100

TS-27

H	-1.13480600	-0.06543900	-0.16551300
Si	-3.32031200	-1.29020500	0.08483600
C	-2.70370100	-2.14693700	1.66517600
H	-3.14216800	-3.14634900	1.78532700
H	-2.95780700	-1.55988800	2.55601400
H	-1.61298100	-2.25526000	1.63850600
C	-2.89853200	-2.40885900	-1.39785100
H	-3.34211600	-3.40769500	-1.28994600
H	-1.81255800	-2.52918900	-1.48760700
H	-3.26563100	-1.98564100	-2.34159800
C	-5.21728600	-1.13641400	0.19624700
H	-5.63448300	-0.72396400	-0.73095200
H	-5.48858700	-0.45255600	1.00897100
H	-5.70429500	-2.10323400	0.38373100
C	-2.80176600	2.49150600	-1.15435100
C	-2.69035500	1.15436300	-1.31338100
C	-2.45465200	0.37014300	-0.09086800
C	-2.62104500	1.27902200	1.06132100
H	-2.14407200	1.10017500	2.02146100
C	1.48320900	-0.04654500	1.67285700
H	0.80392100	-0.78807800	2.11126500
H	2.39667500	-0.02515200	2.28249400
H	0.98125200	0.92469000	1.76134100
C	1.58631900	0.86538400	-1.51222800
H	1.14359200	1.77349200	-1.08455200
H	2.52825500	1.13701400	-2.00737100
H	0.88685400	0.51485200	-2.28031300
C	1.45625600	-2.29540800	-0.69707700
H	0.89595000	-2.31901700	-1.64017800
H	2.38625900	-2.86122700	-0.82655200
H	0.83693200	-2.80303200	0.05282300
Si	1.78661500	-0.48827500	-0.16921100
C	4.30611100	1.57520700	0.48236400
C	4.65824200	0.12025800	0.09867800
H	3.75912700	2.07583300	-0.32217200
H	3.68853500	1.60873800	1.38490800
H	5.22059400	2.15134900	0.67805200
C	5.44568300	-0.52870700	1.25786100
C	5.54191500	0.13616900	-1.16789700
H	5.69569300	-1.56357900	0.99783900
H	6.37640400	0.01158500	1.48098600
H	4.83142400	-0.54989500	2.16511200
H	6.47435500	0.69749500	-1.01566700
H	5.79457400	-0.89144700	-1.45280800
H	4.99560800	0.59111300	-2.00183400
O	3.54667600	-0.69882600	-0.17045900
H	-0.11668500	-0.37150000	-0.19286100
H	-2.71484600	0.69462700	-2.30025300
H	-2.92058700	3.24284500	-1.92649700
S	-2.69677700	2.98703600	0.54360400

TS-28

H	-1.68210500	1.28504000	-0.15474000
Si	-4.59015300	0.92715700	0.41520400
C	-5.42457100	1.76541800	-1.07767300
H	-6.38524500	2.19213900	-0.76095300
H	-5.64574400	1.03536700	-1.86563700
H	-4.83939500	2.57447700	-1.52559100

C	-4.51466600	2.15952900	1.86151800
H	-5.52745700	2.45222700	2.16566000
H	-3.97035000	3.07796000	1.61390600
H	-4.02955900	1.71168500	2.73764000
C	-5.74648300	-0.49434100	0.91790300
H	-5.43440900	-0.95007900	1.86393100
H	-5.74487800	-1.28633800	0.15927100
H	-6.78093400	-0.14632700	1.03370100
O	-0.67806600	1.83246900	-0.34261100
C	-0.83178100	3.26606500	-0.43286700
C	-0.75448200	3.87396200	0.98034400
H	0.23413500	3.70151400	1.42573500
H	-1.51634500	3.42711300	1.62873500
H	-0.91742700	4.95836900	0.96272200
C	0.31366300	3.80945700	-1.29901900
H	0.22386900	3.43700600	-2.33056400
H	1.28045300	3.50657800	-0.88769400
H	0.28838900	4.90452700	-1.34992100
C	-2.16907300	3.63723200	-1.08959700
H	-2.27480300	3.13159200	-2.05590000
H	-2.22118400	4.71863000	-1.26267800
H	-3.01569600	3.35701400	-0.46129600
C	-2.28025800	-1.89375600	-0.68457500
C	-2.10503900	-1.88789400	0.74916500
C	-2.40528500	-0.59030800	1.19073500
C	-2.82978300	0.25765200	0.07516100
H	-2.43071100	-0.27563900	2.22881500
O	1.62647000	-1.10551000	1.68534300
C	1.86779200	-1.57479200	2.98723500
C	1.88039000	-3.12025300	3.00584800
H	2.09942200	-3.52786900	4.00109900
H	0.90844600	-3.51320000	2.68519700
H	2.64613500	-3.49403600	2.31245400
C	3.23743100	-1.06690900	3.49615400
H	3.26976900	0.03031100	3.47585200
H	3.45209000	-1.39318600	4.52184500
H	4.04789800	-1.44209600	2.85461600
C	0.76866500	-1.06817900	3.95001000
H	-0.21906700	-1.36664900	3.58304200
H	0.89094100	-1.45197100	4.97085700
H	0.79207200	0.03109200	4.01188600
O	1.78291700	-1.17024200	-1.55501200
O	2.66795200	1.61061300	0.04622800
C	3.80780000	2.40649500	0.22868300
C	3.55442500	3.47067500	1.32151500
H	3.30483600	2.98046300	2.27243000
H	4.42630900	4.11451900	1.49451900
H	2.71194100	4.11221300	1.03765300
C	4.19958500	3.11506800	-1.08964100
H	5.11635700	3.70998600	-0.98806600
H	4.36540900	2.36959700	-1.87855000
H	3.40035100	3.78759600	-1.42179900
C	5.01382600	1.53728900	0.67458100
H	4.77787300	0.99927600	1.60242400
H	5.27266100	0.80739800	-0.10896100
H	5.91675300	2.13238200	0.85950500
C	2.20833300	-1.76386300	-2.75539700
C	1.44163500	-1.15713200	-3.95394000
H	1.66177800	-0.08187800	-4.04859400
H	1.71088000	-1.62433400	-4.90967800
H	0.36184100	-1.27701600	-3.80556900
C	3.72234500	-1.51901700	-2.96126200
H	4.29662200	-1.98638900	-2.14765800

H	4.09531800	-1.93623900	-3.90533400
H	3.93876200	-0.44229000	-2.95811800
C	1.95344900	-3.28737100	-2.72290000
H	2.29296700	-3.79047700	-3.63736500
H	2.48910500	-3.73771700	-1.87563500
H	0.88324800	-3.49262900	-2.59964900
Na	0.53373300	-2.23123900	0.02454500
Na	0.86015900	1.00183800	1.33499200
Na	1.18780300	1.00514300	-1.54734700
Na	3.13776600	-0.59179800	0.14057800
N	-2.76368300	-0.66852800	-1.06373800
C	-2.81470800	-0.25521800	-2.44637300
H	-3.41102300	-0.95775100	-3.04187600
H	-3.27673100	0.72998600	-2.51303700
H	-1.80916600	-0.20048900	-2.89723700
C	-1.94638600	-3.00412000	-1.46500200
C	-1.49873600	-4.17826100	-0.80553800
C	-1.38910000	-4.21713300	0.59181300
C	-1.68099400	-3.09237000	1.38107800
H	-1.59085800	-3.13961600	2.46235900
H	-1.07502900	-5.13923800	1.07612500
H	-1.26716900	-5.06332200	-1.39150400
H	-2.05963400	-2.98932400	-2.54485500